

## DAFTAR PUSTAKA

- Abedini, A., Khosravi, M., & Calagari, A. A. (2019). Geochemical Characteristics of the Arbanos Karst-Type Bauxite Deposit. NW Iran: Implications for Parental Affinity and Factors Controlling the Distribution of Elements. *Journal of Geochemical Exploration*, 200, 249-265. doi: <https://doi.org/10.1016/j.gexplo.2018.09.004>
- Atakoglu, O. O., & Yalcin, M. G. (2021). Geochemical Characterization of the Sutlegen Bauxite Deposit. *Mining of mineral deposits*, 15.
- Aziz, M., (2010). Ekstraksi Alumina dari Residu Bauksit untuk Bahan Baku Zeolit Sintetis dengan Produk Samping Konsentrat Besi. *Jurnal Zeolit Indonesia*, 9 (2).
- Bardossy, G. (1982). *Karst Bauxites Bauxite Deposits on Carbonate Rocks*. Amsterdam: Elsevier.
- Beiser, A. (1992). *Modernt Technical Physics*. Malang: UB Press.
- Borra, C. R., Blanpain, B., Pontikes, Y., Binnemans, K. & Van Gerven, T. (2016). Recovery of Rare Earths and Other Valuable Metals From Bauxite Residu (Red Mud): A Review. *Journal Of Sustainable Metallurgy*, 2(4), pp. 365-386.
- Calagari, A.A., & Abedini, A. (2007). Geochemical Investigations on Permo-Triassic Bauxite Horizon at Kanisheeteh, East of Bukan, West-Azarbaidjan, Iran. *Journal of Geochemical Exploration*, 94, 1-18.
- Craigh, J. R., & Vaughan. (1981). *Ore Microscopy and Ore Petrography*. USA: John Wiley and Sons.
- Deady, E.A., Mouchos, E., Goodenough, K., Williamson, B.J., & Wall, F. (2016). A Review of the Potential for Rare-Earth Element Resources from European Red Mud: Examples from Seydişehir, Turkey and Parnassus-Giona, Greece. *Mineralogical Magazine*, 80, 43–61.
- Deng, J., Wang, Q., Yang, S., Liu, X., Zhang, Q., Yang, L., and Yang, Y., (2010). Genetic Relationship Between the Emeishan Plume and the Bauxite Deposits in Western Guangxi, China: Constraints from U–Pb and Lu–Hf Isotopes of the Detrital Zircons in Bauxite Ores. *Journal of Asian Earth Sciences*, 37, 412-424.
- Dill, H. G. (2020). A geological and mineralogical review of clay mineral deposits | phyllosilicate ore guides in Central Europe—A function of geodynamics | climate change. *Ore Geology Reviews*, 119, 103304.
- F., 2005. A History of Hydrometallurgy. *Hydrometallurgy*, 79, 15-Elsevier.



- Husein, S., Srijono., & Dyah, H. (2007). *Morfotektonik Pembentukan Kars Maros, Sulawesi Selatan*. Universitas Gadjah Mada: Yogyakarta.
- Hyamn, (2017). Mineral Bauksit. Hyamn.com (Diakses Pada Tanggal 5 April 2024).
- Isbandi, D. (1986). *Mineralogi*. Yogyakarta: Nur Cahaya.
- Jamaludin, A. & Darma A. (2012). Analisis Kerusakan X-Ray Fluoresence (XRF). *Teknologi Bahan Bakar Nuklir*, 9(10), 19-28.
- Jamaluddin. (2010). *XRD (X-Ray Diffractions)*. Kendari: Universitas Haluoleo.
- King, J. R. (2001). *The Aluminium Industry*. Elsevier.
- Lang, A. M., Aasly, K., & Ellefmo, S. L. (2018). Mineral Characterization as a Tool in The Implementation of Geometallurgy Into Industrial Mineral Mining. *Minerals Engineering*, 116, 114–122.
- Liu, L., Liu, X., Yang, S., Zhao, L., Sun, X., & Zhang, J. (2023). Mineralogical and Geochemical Investigations on the Early Permian Yuxi Karstic Bauxite Deposit, Central Yunnan, China. *Ore Geology Reviews*, 153(105296).
- Luo, Z. 2008. Prospective Study of World The Aluminium Industry. Seville: European Communities.
- Mameli, P., Mongelli, G., Oggiano, G., & Dinelli, E. (2007). Geological, Geochemical and Mineralogical Features of Some Bauxite Deposits from Nurra (Western Sardinia, Italy): Insights on Conditions of Formation and Parental Affinity. *International Journal of Earth Sciences*, 96, 887-902.
- Mead, L. J., & Bateman., A.M. (1981). *Economic Mineral Deposits 3rd Edition*. New York: .
- Mo, H., Yang, R., Luo, C., Li, X., Ji, Y., Yang, G., & Zeng, Z. (2023). Effect of Karst Geomorphology on the Sedimentary Mineralization and Geochemical Distribution of Bauxite: An Example from the Xiaoyuan Area in Qingzhen, Guizhou Province. *Minerals*, 13(8), 1013.
- Mongelli, G., Boni, M., Buccione, R., & Sinisi, R. (2014). Geochemistry of the Apulian karst bauxites (southern Italy): chemical fractionation and parental affinities. *Ore Geology Reviews*, 63, 9-21.
- Munasir, M., Triwikantoro, T., Zainuri, M. & Darminto, D. (2012). Uji XRD dan XRF pada Bahan Mineral (Batuan dan Pasir) Sebagai Sumber Material Cerdas ( $\text{CaCO}_3$  DAN  $\text{SiO}_2$ ), *Jurnal Penelitian Fisika dan Aplikasinya PFA*, 2(1), 20–29. doi: 10.26740/jpfa.v2n1.p20-29.
- I., Hein, J.R., & Hanilci, N. (2002). Genesis of the Dogankuzu and Mortas auxite Deposits, Taurides, Turkey: Separation of Al, Fe, and Mn and



- Implications for Passive Margin Metallogeny. *Economic Geology*, 97, 1063-1077.
- Palit, C., & Suliestyah. (2020). Studi Konsentrasi pada Bauksit Asal Tayan dengan Menggunakan Metode Flotasi Kebalikan. *Jurnal Geomine*, 8(2), 121-130.
- Palmer, Sara, J., Frost, R. L., & Nguyen, Tai M. (2009). Hydrotalcites and Their Role in Coordination of Anions in Bayer Liquors: Anion Binding in Layered Double Hydroxides. *Coordination Chemistry Reviews*, 253(1-2), 250-267.
- Radusinovic S., Jelenkovic R., Pacevski A., Simic V., Bozovic D., Holclajtner-Antunovic I., & Zivotic D. (2016). Content and Mode of Occurrences of Rare Earth Elements in the Zagrad Karstic Bauxite Deposit (Niksic Area, Montenegro). *Ore Geology Reviews* (in press).
- Ramadhan, F. R., Aribowo, Y., Widiarso, D. A., & Betraz, A. (2014). Geologi, Karakteristik dan Genesa Endapan Laterit Bauksit PT. Antam (Persero) Tbk, Unit Geomin, Daerah Kenco, Kabupaten Landak, Provinsi Kalimantan Barat. *Geological Engineering E-Journal*, 6(1), 80-95.
- Reddy, B. R. (1997). The Effect of Pretreatment on Magnetic Separation of Ferruginous Minerals in Bauxite. *Journal Magnetic and Electrical Separation*, 8, 115-123.
- Sari, R. P., Arsyad, M., dan Vistarani A. T. (2019). Analisis Mineral Pembentuk Facies Gua Salukang Kallang Kawasan Karst Taman Nasional Bantimurung Bulusaraung Maros. *Jurnal Sains dan Pendidikan Fisika (JSPF)*, 15(3), 78-85.
- Sari, R. K. (2016). Potensi Mineral Batuan Tambang Bukit dengan Metode XRD, XRF, dan AAS. *Eksakta* 2, 13-23.
- Salamab, E. S., Taghipour, B., & Mongelli. G. (2019). Clayey Bauxite from the Irano-Himalayan Belt: Critical Metals Provenance and Palaeoclimate in the Upper Cretaceous Semrom ore deposit. Zagros Mountain, Iran. *Journal of Asian Earth Sciences*, 172, 126-142.
- Scarsella, A. A. (2015). Energy In Alumina Refinery : Settling A New Limits. *Light Metal*, 171-179.
- Senyuta, A. 2013. Innovative Technology for Alumina Production from Low-Grade Raw Material . *Light Metal* 2013, 203-208.
- Shaffer, J.W. (1975). Bauxite Raw Materials. In: *Industrial Minerals and Rocks (Non-Metallic Other Than Fuels)*. *Amer Inst Mining Metall Petroleum Engineering*, 442-459.
- . (2008). Economic Processing of High Silica Bauxites—Existing and Potential Processes. *Australia, Parker Center, CSIRO Light Metals Flagship*.



- Smith, P. (2009). The Processing of High Silica Bauxites Review of Existing and Potential Processes. *Hydrometallurgy*, 98(1), 162-176.
- Sujiono, E. H., Diantoro, M., & Samnur. (2014). Karakterisasi Sifat Fisis Batuan Nikel di Sorowako Sulawesi Selatan. *Pendidikan Fisika Indonesia*, 10(2), 163-167.
- Sukamto, R. A. B., Supriatna, S. A.. M. (1982). *Peta Geologi Lembar Ujung Pandang, Benteng dan Sinjai*. Direktorat Geologi, Departemen Pertambangan Republik Indonesia bekerjasama dengan USGS.
- Sukmawati, Palloan, P., & Arsyad, M. (2015). Karakterisasi Jenis Mineral Ornamen Gua Salukang Kallang dengan Metode X-Ray Diffraction. *Jurnal Sains dan Pendidikan Fisika*, 11(3).
- Sydney, Margery, dan Johnstone, J., 1961. Minerals for the Chemical and allied Industries, Ed. 2<sup>nd</sup>, John Wiley & Sons Inc, New York, USA.
- Utomo, W. P., dan Rosyidah, A. (2010). Sintesis dan Karakterisasi Fasa Aurivillius Lapis Dua  $\text{CaBi}_2\text{Ta}_2\text{O}_9$  Dan  $\text{CaBi}_2\text{Ta}_n\text{BO}_9$ . *Prosiding Tugas Akhir Semester Ganjil 2010/2011*, 5.
- Veleton, I. (1972). *Bauxites*. Amsterdam: Elsevier Publishing Company.
- Wei, X., Ji, H.B., Li, D.J., Zhang, F.L., & Wang, S.J. (2013). Material Source Analysis and Element Geochemical Research About Two Types of Representative Bauxite Deposits and Terra Rossa in Western Guangxi, Southern China. *Journal of Geochemical Exploration*, 133, 68-87.
- Wicaksono, H. H., & Handayani, E. (2021). Karakterisasi Mineralogi Mineral Berbasis Cu-Fe-S dengan SEM EDS di Daerah Kelapa Kampit, Pulau Belitung. *Jurnal Teknologi Mineral Dan Batubara*, 17(1), 27–38. <https://doi.org/10.30556/JTMB.VOL17.NO1.2021.1127>
- Widiyastuti, D. A. (2016). Analisa Struktur Batuan dari Sungai Aranio Kabupaten Banjar Menggunakan X-Ray Difrraction. *Sains dan Terapan Politeknik Hasnur*, 4(1), 8-13.
- Yang, S., Wang, Q., Deng, J., Wang, Y., Kang, W., Liu, X., & Li, Z. (2019). Genesis of Karst Bauxite-Bearing Sequences in Baofeng, Henan (China) and the Distribution of Critical Metals. *Ore Geology Reviews*, 115(103161).
- Zarasvandi, A., Charchi, A., Carranza, E. J. M., & Alizadeh, B. (2008). Karst Bauxite Deposits in the Zagros Mountain Belt, Iran. *Ore Geology Reviews*, 34(4), 521-532



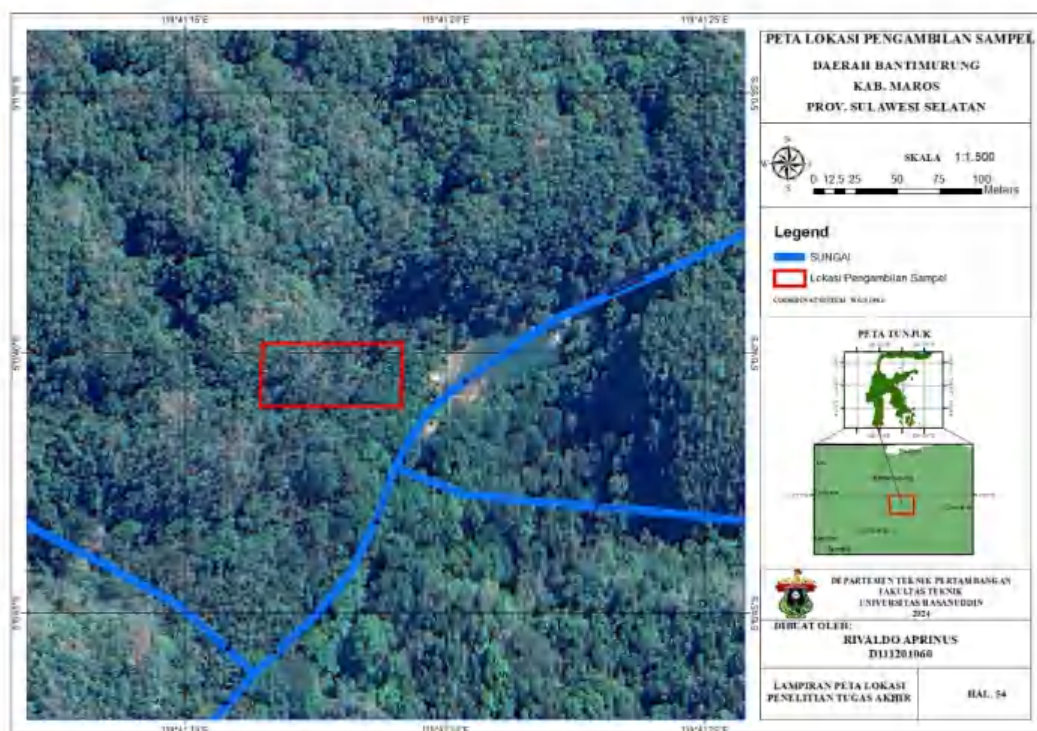
## LAMPIRAN



Optimized using  
trial version  
[www.balesio.com](http://www.balesio.com)

## Lampiran 1 Peta Pengambilan Sampel





## Lampiran 2 Hasil Mikroskopis



Optimized using  
trial version  
[www.balesio.com](http://www.balesio.com)



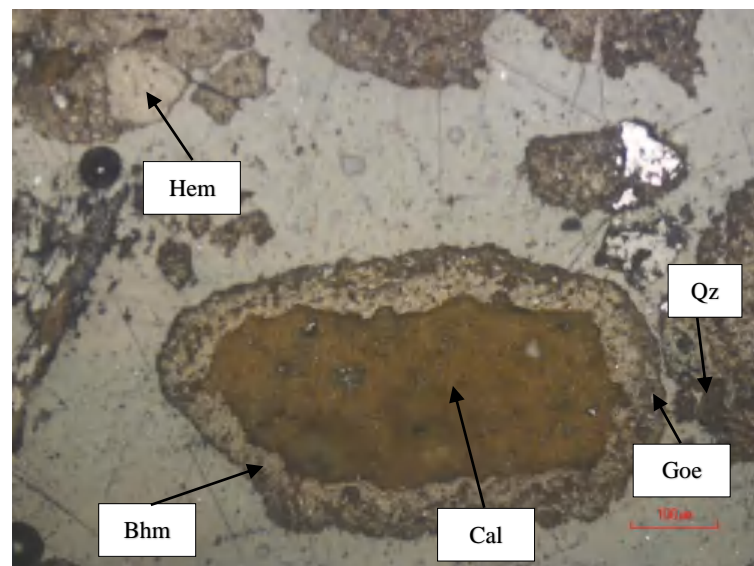
<b>Lokasi</b> : Bantimurung, Kabupaten Maros		<b>Kode Sampel</b> :RBTM 2
<b>Mineral Bijih</b> : Boehmite		
<b>Mineral Pengotor:</b> Goetit, Hematit, Kuarsa, dan Kalsit		
<b>Referensi</b> :(Kontak, 2005), (Warr, 2021)		
<b>Deskripsi Mineralogi</b>		
<b>Komposisi Mineral</b>	<b>Simbol</b>	<b>Keterangan optik mineral</b>
<b>Goetit</b>	<b>(Goe)</b>	Sistem kristal ortorombik, berwarna abu-abu gelap dengan bentuk (subhedral), ukuran mineral yang tampak yaitu 50 $\mu\text{m}$ -250 $\mu\text{m}$ .
<b>Hematit</b>	<b>(Hem)</b>	Sistem kristal trigonal, berwarna abu-abu terang dengan bentuk (anhedral-subhedral), ukuran mineral yang tampak yaitu 10 $\mu\text{m}$ -100 $\mu\text{m}$
<b>Kuarsa</b>	<b>(Qz)</b>	Sistem kristal trigonal, berwarna hitam dengan bentuk (anhedral-subhedral), ukuran mineral yang tampak yaitu 20 $\mu\text{m}$ -50 $\mu\text{m}$
<b>Boehmite</b>	<b>(Bhm)</b>	Sistem Kristal ortorombik, berwarna coklat pucat dengan bentuk (anhedral-subhedral), ukuran mineral yang tampak yaitu 50 $\mu\text{m}$ -100 $\mu\text{m}$ .
<b>Kalsit</b>	<b>(Cal)</b>	Sistem kristal heksagonal, berwarna kuning kecoklatan dengan bentuk (anhedral-subhedral), ukuran mineral yang tampak yaitu 50 $\mu\text{m}$ -100 $\mu\text{m}$ .
<b>Foto</b>		



<b>Lokasi</b> : Bantimurung, Kabupaten Maros		<b>Kode Sampel</b> :R-BTM 2
<b>Mineral Bijih</b> : Boehmite		
<b>Mineral Pengotor</b> : Goetit, Hematit, Kuarsa, dan Kalsit		
<b>Referensi</b> :(Kontak, 2005), (Warr, 2021)		
<b>Deskripsi Mineralogi</b>		
<b>Komposisi Mineral</b>	<b>Simbol</b>	<b>Keterangan optik mineral</b>
<b>Goetit</b>	<b>(Goe)</b>	Sistem kristal ortorombik, berwarna abu-abu gelap dengan bentuk (subhedral), ukuran mineral yang tampak yaitu 50 $\mu\text{m}$ -250 $\mu\text{m}$ .
<b>Hematit</b>	<b>(Hem)</b>	Sistem kristal trigonal, berwarna abu-abu terang dengan bentuk (anhedral-subhedral), ukuran mineral yang tampak yaitu 10 $\mu\text{m}$ -100 $\mu\text{m}$
<b>Kuarsa</b>	<b>(Qz)</b>	Sistem kristal trigonal, berwarna hitam dengan bentuk (anhedral-subhedral), ukuran mineral yang tampak yaitu 20 $\mu\text{m}$ -50 $\mu\text{m}$
<b>Boehmite</b>	<b>(Bhm)</b>	Sistem Kristal ortorombik, berwarna coklat pucat dengan bentuk (anhedral-subhedral), ukuran mineral yang tampak yaitu 50 $\mu\text{m}$ -100 $\mu\text{m}$ .
<b>Foto</b>		
<p>The image shows a microscopic view of mineral grains. Four labels with arrows point to specific features: 'Qz' points to a dark, irregularly shaped grain; 'Hem' points to a smaller, lighter-colored grain; 'Goe' points to a large, dark, elongated grain; and 'Bhm' points to a large, light-colored, irregularly shaped grain.</p>		



<b>Lokasi</b> : Bantimurung, Kabupaten Maros		<b>Kode Sampel</b> :R-BTM 2
<b>Mineral Bijih</b> : Boehmite		
<b>Mineral Pengotor</b> : Goetit, Hematit, Kuarsa, dan Kalsit		
<b>Referensi</b> : (Kontak, 2005), (Warr, 2021)		
<b>Deskripsi Mineralogi</b>		
Komposisi Mineral	Simbol	Keterangan optik mineral
Goetit	(Goe)	Sistem kristal ortorombik, berwarna abu-abu gelap dengan bentuk (subhedral), ukuran mineral yang tampak yaitu 50 $\mu\text{m}$ -250 $\mu\text{m}$ .
Hematit	(Hem)	Sistem kristal trigonal, berwarna putih abu-abu terang dengan bentuk (anhedral-subhedral), ukuran mineral yang tampak yaitu 10 $\mu\text{m}$ -100 $\mu\text{m}$
Kuarsa	(Qz)	Sistem kristal trigonal, berwarna hitam dengan bentuk (anhedral-subhedral), ukuran mineral yang tampak yaitu 20 $\mu\text{m}$ -50 $\mu\text{m}$
Boehmite	(Bhm)	Sistem Kristal ortorombik, berwarna coklat pucat dengan bentuk (anhedral-subhedral), ukuran mineral yang tampak yaitu 50 $\mu\text{m}$ -100 $\mu\text{m}$ .
Kalsit	(Cal)	Sistem kristal heksagonal, berwarna kuning kecoklatan dengan bentuk (anhedral-subhedral), ukuran mineral yang tampak yaitu 50 $\mu\text{m}$ -100 $\mu\text{m}$ .

**Foto**

<b>Lokasi</b> : Bantimurung, Kabupaten Maros		<b>Kode Sampel</b> :R-BTM 2
<b>Mineral Bijih</b> : Boehmite		
<b>Mineral Pengotor</b> : Goetit, Hematit, Kuarsa, dan Kalsit		
<b>Referensi</b> : (Kontak, 2005), (Warr, 2021)		
<b>Deskripsi Mineralogi</b>		
<b>Komposisi Mineral</b>	<b>Simbol</b>	<b>Keterangan optik mineral</b>
<b>Goetit</b>	<b>(Goe)</b>	Sistem kristal ortorombik, berwarna abu-abu gelap dengan bentuk (subhedral), ukuran mineral yang tampak yaitu 50 $\mu\text{m}$ -250 $\mu\text{m}$ .
<b>Hematit</b>	<b>(Hem)</b>	Sistem kristal trigonal, berwarna abu-abu terang dengan bentuk (anhedral-subhedral), ukuran mineral yang tampak yaitu 10 $\mu\text{m}$ -100 $\mu\text{m}$
<b>Kuarsa</b>	<b>(Qz)</b>	Sistem kristal trigonal, berwarna hitam dengan bentuk (anhedral-subhedral), ukuran mineral yang tampak yaitu 20 $\mu\text{m}$ -50 $\mu\text{m}$
<b>Boehmite</b>	<b>(Bhm)</b>	Sistem Kristal ortorombik, berwarna coklat pucat dengan bentuk (anhedral-subhedral), ukuran mineral yang tampak yaitu 50 $\mu\text{m}$ -100 $\mu\text{m}$ .
<b>Kalsit</b>	<b>(Cal)</b>	Sistem kristal heksagonal, berwarna kuning kecoklatan dengan bentuk (anhedral-subhedral), ukuran mineral yang tampak yaitu 50 $\mu\text{m}$ -100 $\mu\text{m}$ .
<b>Foto</b>		



## Lampiran 3 Hasil Analisis XRD



# Match! Phase Analysis Report

## SAMPLE: R-BTM-1 (5-70)

### Sample Data

File name	R-BTM-1.RAW
File path	F:/RIVALDO XRD/R-BTM-1
Data collected	Mar 21, 2024 12:09:18
Data range	5.000° - 70.000°
Original data range	5.000° - 70.000°
Number of points	3251
Step size	0.020
Rietveld refinement converged	No
Alpha2 subtracted	No
Background subtr.	No
Data smoothed	Yes
Radiation	X-rays
Wavelength	1.540600 Å

### MATCHED PHASES

Index	Amount (%)	Name	Formula sum
A	28.8	Boehmite	Al H O2
B	22.7	Kaolinite	Al2 O9 Si2
C	22.0	Goethite	Fe H O2
D	18.1	Calcite	C Ca O3
E	5.6	Hematite	Fe2 O3
F	3.0	Quartz	O2 Si
	8.9	Unidentified peak area	

#### A: Boehmite (28.8 %)\*

Formula sum	Al H O2
Entry number	96-901-2254
Figure-of-Merit (FoM)	0.808476*
Total number of peaks	50
Peaks in range	23
Peaks matched	12
Intensity scale factor	0.65*
Space group	C m c m
Crystal system	orthorhombic
Unit cell	a= 2.8678 Å b= 12.2188 Å c= 3.6941 Å
l/lc	2.76
Calc. density	3.078 g/cm <sup>3</sup>
Reference	Bokhimi X., Toledo-Antonio J A, Guzman-Castillo M L, Hernandez-Beltran F, "Relationship between crystallitesize and bond lengths in boehmiteLocality: syntheticSample: preparation T = 240 C", Journal of Solid State Chemistry <b>159</b> , 32-40 (2001)

#### B: Kaolinite (22.7 %)\*



m	Al2 O9 Si2
er	96-901-5000
erit (FoM)	0.828320*
er of peaks	264
nge	119

Peaks matched	73
Intensity scale factor	0.22 <sup>*</sup>
Space group	C 1 c 1
Crystal system	monoclinic
Unit cell	a= 5.1480 Å b= 8.9200 Å c= 14.5350 Å β= 100.200 °
I/lc	1.17
Calc. density	2.570 g/cm <sup>3</sup>
Reference	Referensi Gruner W., "The Crystal Structure of Kaolinite_cod_database_code 1011045", Zeitschrift fur Kristallographie <b>83</b> ,75-88 (1932)

### C: Goethite (22.0 %)\*

Formula sum	Fe H O2
Entry number	96-900-2159
Figure-of-Merit (FoM)	0.771754 <sup>*</sup>
Total number of peaks	86
Peaks in range	35
Peaks matched	24
Intensity scale factor	0.53 <sup>*</sup>
Space group	P n m a
Crystal system	orthorhombic
Unit cell	a= 9.9134 Å b= 3.0128 Å c= 4.5800 Å
I/lc	2.93
Calc. density	4.314 g/cm <sup>3</sup>
Reference	Gualtieri A., Venturelli P., "In situ study of the goethite-hematite phase transformation by real timesynchrotron powder diffractionSample at T = 25 C", American Mineralogist <b>84</b> , 895-904 (1999)

### D: Calcite (18.1 %)\*

Formula sum	C Ca O3
Entry number	96-900-7690
Figure-of-Merit (FoM)	0.869666 <sup>*</sup>
Total number of peaks	43
Peaks in range	18
Peaks matched	13
Intensity scale factor	0.52 <sup>*</sup>
Space group	R -3 c
Crystal system	trigonal (hexagonal axes)
Unit cell	a= 4.9880 Å c= 17.0680 Å
I/lc	3.53
Calc. density	2.712 g/cm <sup>3</sup>
Reference	Referensi Maslen E. N., Streltsov V. A., Streltsova N. "Electron density and optical anisotropy in rhombohedral carbonates.III. Synchrotron X-ray studies of CaCO <sub>3</sub> , MgCO <sub>3</sub> and MnCO <sub>3</sub> ", Acta Crystallographica, Section B <b>51(6)</b> , 929-939 (1995)
R., Ishizawa N.,	

### E: Hematite (5.6 %)\*

Formula sum	Fe2 O3
Entry number	96-900-0140
Figure-of-Merit (FoM)	0.738696 <sup>*</sup>
Total number of peaks	34
Peaks in range	14
Peaks matched	11
Intensity scale factor	0.18 <sup>*</sup>
Space group	R -3 c
Crystal system	trigonal (hexagonal axes)
Unit cell	a= 5.0380 Å c= 13.7720 Å
I/lc	3.97
Calc. density	5.256 g/cm <sup>3</sup>



Reference  
L. W.,

Referensi Blake R. L., Hessevick R. E., Zoltai T., Finger  
"Refinement of the hematite structure", American Mineralogist  
**51**, 123-129 (1966)

## F: Quartz (3.0 %)\*

Formula sum	O2 Si
Entry number	96-900-5018
Figure-of-Merit (FoM)	0.741315*
Total number of peaks	35
Peaks in range	16
Peaks matched	9
Intensity scale factor	0.08*
Space group	P 32 2 1 S
Crystal system	trigonal (hexagonal axes)
Unit cell	a= 4.9137 Å c= 5.4047 Å
I/lc	3.31
Calc. density	2.649 g/cm <sup>3</sup>
Reference dependence of	Referensi Kihara K., "An X-ray study of the temperature the quartz structureSample: at T = 298 K", European Journal of Mineralogy <b>2</b> , 63-77 (1990)

(\*): 2theta values have been shifted internally for the calculation of the amounts, the intensity scaling factors as well as the figure-of-merit (FoM), due to the active search-match option 'Automatic zero point adaption'.

## CANDIDATES

Name	Formula	Entry No.	FoM
	Pd2 Sn Tm	96-152-2426	0.8113
aluminum phosphate	Al O4 P	96-201-0796	0.8112
Silver indium (0.75/0.25) – HT	Ag0.75 In0.25	96-231-0021	0.8092
	C2 Mn N2	96-432-8522	0.8058
	Er Rh	96-231-0286	0.8018
Tridymite	O2 Si	96-901-3394	0.7986
Li4 Ti0.8 N2.4 (Li2 O)1.6	Li7.2 N2.4 O1.6 Ti0.8	96-153-7482	0.7982
Tridymite	O2 Si	96-901-3492	0.7972
	Pd2 Sn Tb	96-152-3489	0.7955
Tridymite	O2 Si	96-901-3493	0.7952
Calcium cadmium oxide (.50/.50/1)	Ca0.5 Cd0.5 O	96-101-0885	0.7916
Tridymite	O2 Si	96-900-0521	0.7915
(Ho3 N) In	Ho3 In N	96-153-3900	0.7911
(Ag2 Al)0.66	Ag1.334 Al0.666	96-150-9590	0.7869
Silver oxide	Ag2 O	96-101-0605	0.7861
	Cu2 In Nd	96-152-8013	0.7854
Zirconium carbide	Zr C	96-101-1323	0.7849
Dilithium Oxide	Li2 O	96-151-4095	0.7836
Potassium aluminium silicate hydroxide * (Muscovite 2M1)	Al3 H2 K O12 Si3	96-101-1050	0.7830
Potassium aluminium silicate hydroxide * (Muscovite 2M1)	Al3 H K O12 Si3	96-110-0014	0.7830
Cu3 Te O6	Cu3 O6 Te	96-210-6307	0.7829
	Pd2 Sn Y	96-152-3934	0.7817
Cu3 Te O6	Cu3 O6 Te	96-153-7440	0.7810
	Dy In Pd2	96-152-4286	0.7808
	Dy Pd2 Sn	96-152-5418	0.7808
	Li	96-900-8505	0.7793
	Li	96-901-1004	0.7793
anium iron(III) antimony oxide (3/0.96/0.98/1/9.12)Cu3 Fe0.98 O9.12 Sb Ti0.9696-100-1690	Cu3 Fe0.98 O9.12 Sb Ti0.9696-100-1690	96-100-1690	0.7787
5 Y0.25) In	Au2 Ce0.75 In Y0.25	96-151-0378	0.7773
	Lu N	96-900-8671	0.7769
realuminiumchloride	C16 Al Cl N16 S4	96-430-9965	0.7766
	Cr2 Li14 N8 O	96-431-1893	0.7759





Europium	Eu	96-900-8535	0.7755
Mg7 Ti H12.7	H12.7 Mg7 Ti	96-153-2668	0.7753
(Cu0.5 Zn0.5) Tb	Cu0.5 Tb Zn0.5	96-152-4032	0.7748
	In Te	96-153-7672	0.7744
Ce (Sn0.5 Ti0.5)3	Ce Sn1.5 Ti1.5	96-152-7970	0.7743
	Cu2 Ni O6 Te	96-810-1058	0.7740
	Ag2 In Sc	96-150-9651	0.7732
Rb Ca H3	Ca H3 Rb	96-153-8968	0.7727
(F2 (N H3)4 Co) (Cl O4)	Cl Co F2 H12 N4 O4	96-154-1243	0.7726
	Ca3 Ge N	96-152-7232	0.7711
	Hf	96-152-2790	0.7708
U Zr N2	N2 U Zr	96-153-8284	0.7692
Arsenolite	As4 O6	96-451-3584	0.7681
	F6 In K Rb2	96-152-9483	0.7678
Calcium oxide (Lime)	Ca O	96-101-1328	0.7670
	O4 Sb0.92 V1.08	96-210-1705	0.7669
Ti O2	O2 Ti	96-153-0151	0.7668
Hydronium pentaquacopper(II) triperchlorate	Cl3 Cu H13 O18	96-220-2293	0.7646
	C2 N2 Zn	96-411-9771	0.7645
(Ce0.2 Y0.8) Zn	Ce0.2 Y0.8 Zn	96-152-5093	0.7636
<b>and 9950 others..</b>			

## Search-Match

### Settings

Reference database used	COD-Inorg REV248644 2020.03.03
Automatic zeropoint adaptation	Yes
Minimum figure-of-merit (FoM)	0.50
2theta window for peak corr.	0.30 deg.
Minimum rel. int. for peak corr.	1
Parameter/influence 2theta	0.50
Parameter/influence intensities	0.50
Parameter multiple/single phase(s)	0.50

## CRITERIA FOR ENTRIES ADDED BY USER

### Reference:

**Entry number:** 96-900-0863;96-900-9156;96-901-2274;96-901-2275;96-901-2276;96-901-5089;96-100-8767;96-100-8768;96-100-8769;96-101-1088;96-221-1653;96-900-2159;96-900-2160;96-900-3077;96-900-3078;96-900-3079;96-900-3080;96-900-3081;96-901-0407;96-901-0408;96-901-0409;96-901-0410;96-901-0411;96-901-1413;96-901-5697;96-901-6060;96-901-6179;96-901-6407;96-101-1046;96-155-0599;96-900-9231;96-900-9235;96-901-5000

## PEAK LIST



<i>theta</i> [°]	<i>d</i> [Å]	<i>I/I0</i>	<i>FWHM</i>	<i>Matched</i>
2.15	7.2768	95.16	0.2400	B
4.47	6.1179	678.82	0.4000	A
8.56	4.7756	207.57	0.3600	
9.94	4.4492	239.68	0.6000	B
0.28	4.3748	251.56	1.2800	B

6	20.62	4.3041	263.70	1.9600	
7	21.06	4.2150	313.88	1.6800	B,F
8	21.28	4.1720	415.82	0.8400	C
9	21.78	4.0773	235.83	0.3600	
10	22.18	4.0047	99.40	2.2000	B
11	22.94	3.8735	152.08	0.4400	
12	23.16	3.8374	104.86	0.3200	D
13	23.50	3.7826	137.97	0.3200	B
14	24.40	3.6452	132.89	0.8800	E
15	24.79	3.5881	163.58	1.2800	B
16	25.22	3.5278	196.06	0.6800	B
17	25.80	3.4501	102.01	0.3600	
18	26.62	3.3462	131.03	0.4000	C,F
19	26.80	3.3239	110.90	0.4000	
20	27.52	3.2387	405.32	0.4000	B
21	28.17	3.1650	628.69	0.3200	A
22	29.44	3.0319	1000.00	0.2800	B,D
23	32.42	2.7594	54.95	0.3220	
24	33.08	2.7054	140.65	0.4400	E
25	33.54	2.6697	144.28	0.4800	C
26	34.86	2.5716	157.66	0.2400	B,C
27	35.19	2.5483	260.77	0.8000	
28	35.60	2.5198	352.74	0.6400	B,C,E
29	36.02	2.4911	472.77	0.4000	B,C,D
30	37.08	2.4228	315.63	1.4400	B,C
31	37.66	2.3864	191.35	2.0800	B
32	38.34	2.3457	782.51	0.3600	A,B
33	39.44	2.2831	287.27	0.2800	C,D,E,F
34	39.88	2.2589	95.65	0.2800	B,C
35	41.26	2.1862	95.91	1.2800	B,C
36	41.61	2.1685	107.21	0.5200	
37	43.20	2.0923	181.96	0.2800	B,C,D,E
38	45.04	2.0112	57.34	0.6115	B,C
39	45.82	1.9788	55.10	0.6178	A,B,F
40	47.53	1.9114	228.59	0.3200	B,C,D
41	48.04	1.8924	96.77	0.4800	B
42	48.45	1.8772	194.01	0.2400	C,D
43	48.91	1.8606	432.70	0.8800	A,B
44	49.24	1.8490	302.47	0.4000	A,E
45	53.64	1.7073	125.40	0.4000	C
46	54.09	1.6940	179.71	1.0800	E
47	54.40	1.6852	147.02	1.8400	B,C
48	55.07	1.6663	183.06	0.8000	A,B,F
49	56.68	1.6227	48.27	0.5800	B,D
50	57.43	1.6033	159.61	0.3600	B,C,D,E,F
51	60.67	1.5252	96.32	0.6000	A,B,D
52	61.44	1.5079	77.06	0.6000	B,C,D
53	62.25	1.4902	170.85	0.6000	A,B,E
54	62.60	1.4827	136.13	1.4000	B
55	63.10	1.4721	98.12	2.7600	B,C,D
56	63.54	1.4630	89.23	3.2400	C
57	64.03	1.4529	234.74	0.3600	A,B,E,F
58	64.34	1.4468	130.40	0.4400	C
59	64.78	1.4379	213.43	0.4800	A,B,C,D
60	67.78	1.3815	54.45	0.2720	A,B,C,F



## Integrated Profile Areas

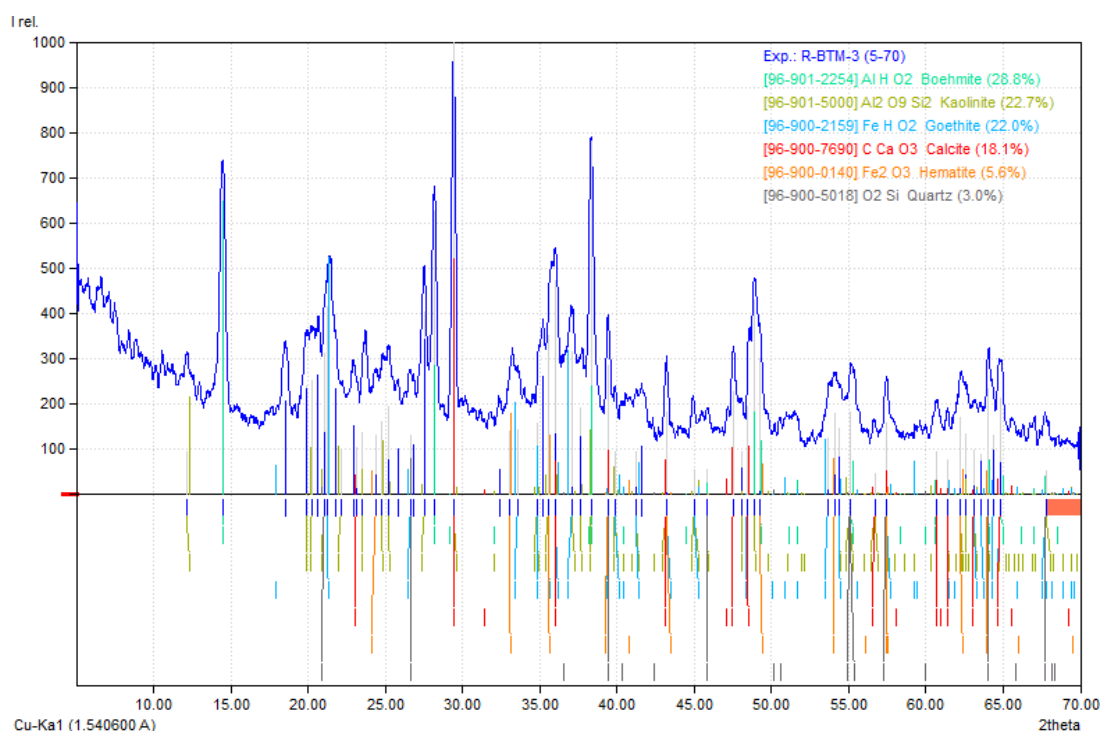
### Based on calculated profile

<b>Profile area</b>	<b>Counts</b>	<b>Amount</b>
Overall diffraction profile	117883	100.00%
Background radiation	82113	69.66%
Diffraction peaks	35770	30.34%
Peak area belonging to selected phases	25332	21.49%
Peak area of phase A (Boehmite)	6310	5.35%
Peak area of phase B (Kaolinite)	5066	4.30%
Peak area of phase C (Goethite)	6758	5.73%
Peak area of phase D (Calcite)	4379	3.71%
Peak area of phase E (Hematite)	2321	1.97%
Peak area of phase F (Quartz)	497	0.42%
Unidentified peak area	10437	8.85%

## PEAK RESIDUALS

<b>Peak data</b>	<b>Counts</b>	<b>Amount</b>
Overall peak intensity	1417	100.00%
Peak intensity belonging to selected phases	1082	76.36%
Unidentified peak intensity	335	23.64%

## Diffraction Pattern Graphics



Match! Copyright © 2003-2020 CRYSTAL IMPACT, Bonn, Germany



Optimized using  
trial version  
[www.balesio.com](http://www.balesio.com)

# Match! Phase Analysis Report

## Sample: R-BTM-2

### Sample Data

File name R-BTM-2.txt  
 File path D:/RIVALDO XRD/R-BTM-2  
 Data collected Mar 21, 2024 12:09:18  
 Data range 5.000° - 70.000°  
 Original data range 5.000° - 70.000°  
 Number of points 3251  
 Step size 0.020  
 Rietveld refinement converged No  
 Alpha2 subtracted No  
 Background subtr. No  
 Data smoothed Yes  
 Radiation X-rays  
 Wavelength 1.541874 Å

### Matched Phases

Index	Amount (%)	Name	Formula sum
A	46.0	Boehmite	Al H O2
B	21.1	Kaolinite	Al2 O9 Si2
C	17.5	Goethite	Fe O2
D	7.0	Hematite	Fe2 O3
E	5.1	Quartz	O2 Si
F	3.3	Calcite	C Ca0.936 Mg0.064 O3
	9.3	Unidentified peak area	

#### A: Boehmite (46.0 %)

Formula sum Al H O2  
 Entry number 96-901-2254  
 Figure-of-Merit (FoM) 0.793751  
 Total number of peaks 100  
 Peaks in range 45  
 Peaks matched 18  
 Intensity scale factor 0.23  
 Space group C m c m  
 Crystal system orthorhombic  
 Unit cell a= 2.8678 Å b= 12.2188 Å c= 3.6941 Å  
 I/lc 2.76  
 Calc. density 3.078 g/cm<sup>3</sup>  
 Reference Bokhimi X., Toledo-Antonio J A, Guzman-Castillo M L, Hernandez-Beltran F, "Relationship between crystallite size and bond lengths in boehmite Locality: synthetic Sample: preparation T = 240 C", Journal of Solid State Chemistry **159**, 32-40 (2001)

#### B: Kaolinite (21.1 %)

Formula sum Al2 O9 Si2  
 Entry number 96-901-5000  
 Figure-of-Merit (FoM) 0.512677  
 Total number of peaks 528  
 Peaks in range 234  
 Peaks matched 92  
 Intensity scale factor 0.05  
 Space group C 1 c 1  
 Crystal system monoclinic  
 Unit cell a= 5.1480 Å b= 8.9200 Å c= 14.5350 Å  $\beta$ = 100.200 °  
 I/lc 1.17  
 Calc. density 2.570 g/cm<sup>3</sup>  
 Reference Gruner W., "The Crystal Structure of Kaolinite\_cod\_database\_code 1011045", Zeitschrift fur



Kristallographie **83**,75-88 (1932)**C: Goethite (17.5 %)**

Formula sum	Fe O2
Entry number	96-901-1413
Figure-of-Merit (FoM)	0.687616
Total number of peaks	174
Peaks in range	71
Peaks matched	34
Intensity scale factor	0.11
Space group	P b n m
Crystal system	orthorhombic
Unit cell	a= 4.5900 Å b= 10.0000 Å c= 3.0300 Å
l/c	3.26
Calc. density	4.195 g/cm <sup>3</sup>
Reference	Hoppe W., "Über die kristallstruktur von alpha-AlOOH (diaspore) und alpha-FeOOH(nadeleisenerz) Locality: Synthetic", Zeitschrift für Kristallographie <b>103</b> , 73-89 (1940)

**D: Hematite (7.0 %)**

Formula sum	Fe <sub>2</sub> O <sub>3</sub>
Entry number	96-901-5965
Figure-of-Merit (FoM)	0.675549
Total number of peaks	68
Peaks in range	28
Peaks matched	12
Intensity scale factor	0.05
Space group	R -3 c
Crystal system	trigonal (hexagonal axes)
Unit cell	a= 5.0346 Å c= 13.7473 Å
l/c	4.02
Calc. density	5.272 g/cm <sup>3</sup>
Reference	Finger L. W., Hazen R. M., "Crystal structure and isothermal compression of Fe <sub>2</sub> O <sub>3</sub> , Cr <sub>2</sub> O <sub>3</sub> , and V <sub>2</sub> O <sub>3</sub> to 50kbars Note: P = 0.001 kbar", Journal of Applied Physics <b>51</b> , 5362-5367 (1980)

**E: Quartz (5.1 %)**

Formula sum	O <sub>2</sub> Si
Entry number	96-900-0779
Figure-of-Merit (FoM)	0.662682
Total number of peaks	66
Peaks in range	28
Peaks matched	10
Intensity scale factor	0.03
Space group	P 3 <sub>2</sub> 2 1 S
Crystal system	trigonal (hexagonal axes)
Unit cell	a= 4.7390 Å c= 5.2790 Å
l/c	3.18
Calc. density	2.915 g/cm <sup>3</sup>
Reference	Levien L., Prewitt C. T., Weidner D. J., "Structure and elastic properties of quartz at pressure P = 48.6 kbar", American Mineralogist <b>65</b> , 920-930 (1980)

**F: Calcite (3.3 %)**

Formula sum	C Ca <sub>0.936</sub> Mg <sub>0.064</sub> O <sub>3</sub>
Entry number	96-900-1298
Figure-of-Merit (FoM)	0.628702
Total number of peaks	86
Peaks in range	36
Peaks matched	13
Intensity scale factor	0.02
Space group	R -3 c



Crystal system	trigonal (hexagonal axes)
Unit cell	a= 4.9673 Å c= 16.9631 Å
I/lc	3.35
Calc. density	2.723 g/cm <sup>3</sup>
Reference	Paquette J., Reeder R. J., "Single-crystal X-ray structure refinements of two biogenic magnesian calcite crystal sample LS", American Mineralogist <b>75</b> , 1151-1158 (1990)

### Candidates

<b>Name</b>	<b>Formula</b>	<b>Entry No.</b>	<b>FoM</b>
Tridymite	O <sub>2</sub> Si	96-901-3394	0.8312
Retgersite	Ni O <sub>10</sub> S	96-901-1290	0.8005
Retgersite	H <sub>12</sub> Ni O <sub>10</sub> S	96-901-1266	0.7948
Nickel sulfate(VI) hexahydrate (Retgersite)	H <sub>12</sub> Ni O <sub>10</sub> S	96-101-1190	0.7924
	Au Cs	96-151-7938	0.7887
	H <sub>12</sub> Ni O <sub>10</sub> S	96-901-1885	0.7857
Retgersite (deuterated)	D <sub>12</sub> Ni O <sub>10</sub> S	96-901-1063	0.7834
Retgersite (deuterated)	D <sub>12</sub> Ni O <sub>10</sub> S	96-901-1265	0.7829
	B N	96-151-1243	0.7820
Retgersite	H <sub>12</sub> Ni O <sub>10</sub> S	96-901-1244	0.7817
Retgersite	H <sub>12</sub> Ni O <sub>10</sub> S	96-901-1079	0.7791
Retgersite	H <sub>12</sub> Ni O <sub>10</sub> S	96-901-1367	0.7788
Boehmite	Al H O <sub>2</sub>	96-901-2254	0.7773
Bohmite	Al H <sub>0.08</sub> O <sub>2</sub>	96-901-5089	0.7766
Retgersite	H <sub>12</sub> Ni O <sub>10</sub> S	96-901-1289	0.7761
aluminum phosphate	Al O <sub>4</sub> P	96-201-0796	0.7736
Boehmite	Al H O <sub>2</sub>	96-901-2253	0.7735
Boehmite	Al H O <sub>2</sub>	96-901-2252	0.7699
Bohmite	Al H O <sub>2</sub>	96-901-2276	0.7693
Alum-(Na)	Al H <sub>24</sub> Na O <sub>20</sub> S <sub>2</sub>	96-901-1066	0.7681
Bohmite	Al H O <sub>2</sub>	96-901-2274	0.7680
Al O (O H) <sub>0.326</sub> (O D) <sub>0.674</sub>	Al D <sub>0.674</sub> H <sub>0.326</sub> O <sub>2</sub>	96-153-6112	0.7638
	Zn Zr	96-152-7719	0.7634
Bohmite	Al H O <sub>2</sub>	96-901-2275	0.7625
I F <sub>7</sub>	F <sub>7</sub> I	96-231-0566	0.7504
Boehmite	Al H O <sub>2</sub>	96-901-2251	0.7501
	C <sub>18</sub> F <sub>10</sub> S <sub>2</sub>	96-150-4619	0.7499
Sodium alum	Al H <sub>24</sub> Na O <sub>20</sub> S <sub>2</sub>	96-901-1065	0.7488
	Al <sub>1.75</sub> Na <sub>1.75</sub> O <sub>4</sub> Si <sub>0.25</sub>	96-200-2894	0.7479
Porphyrazinealuminiumchloride	C <sub>16</sub> Al Cl N <sub>16</sub> S <sub>4</sub>	96-430-9965	0.7465
Boehmite	Al H O <sub>2</sub>	96-901-2250	0.7452
(Hf Mo)	Hf Mo	96-152-2747	0.7440
(Mo <sub>0.1</sub> Nb <sub>0.45</sub> U <sub>0.45</sub> )	Mo <sub>0.1</sub> Nb <sub>0.45</sub> U <sub>0.45</sub>	96-152-3208	0.7421
Pd <sub>2</sub> Sn (Y <sub>0.7</sub> Yb <sub>0.3</sub> )	Pd <sub>2</sub> Sn Y <sub>0.7</sub> Yb <sub>0.3</sub>	96-152-2428	0.7417
	Ir Tm	96-231-0188	0.7409
	C <sub>8</sub> H <sub>14</sub> O <sub>10</sub> S <sub>2</sub>	96-200-9750	0.7402
(Ni (N H <sub>3</sub> )) (C N) <sub>2</sub> (H <sub>2</sub> O) <sub>.25</sub>	C <sub>2</sub> H <sub>3.5</sub> N <sub>3</sub> Ni O <sub>0.25</sub>	96-153-8520	0.7396
Silicon oxide (Cristobalite high)	O <sub>2</sub> Si	96-101-0922	0.7393
	Sc Zn	96-152-7720	0.7393
Potassium aluminium silicate hydroxide * (Muscovite 2M1)	Al <sub>3</sub> H <sub>2</sub> K O <sub>12</sub> Si <sub>3</sub>	96-101-1050	0.7392
Potassium aluminium silicate hydroxide * (Muscovite 2M1)	Al <sub>3</sub> H K O <sub>12</sub> Si <sub>3</sub>	96-110-0014	0.7392
Tridymite	O <sub>2</sub> Si	96-900-5271	0.7391
	C <sub>2</sub> Mn N <sub>2</sub>	96-432-8522	0.7388
	Nb	96-400-1054	0.7381
Brushite (deuterated)	Ca D <sub>5</sub> O <sub>6</sub> P	96-900-7300	0.7376
Brushite (deuterated)	Ca D <sub>5</sub> O <sub>6</sub> P	96-900-7289	0.7375
	Nb	96-400-0951	0.7374
	H <sub>12</sub> Ni O <sub>10</sub> Se	96-152-7380	0.7373
	Ca D <sub>5</sub> O <sub>6</sub> P	96-900-7299	0.7369
	Ca D <sub>5</sub> O <sub>6</sub> P	96-900-7288	0.7367
	Er <sub>0.4</sub> Pd <sub>2</sub> Sn Y <sub>0.6</sub>	96-152-4844	0.7366
	Ca D <sub>5</sub> O <sub>6</sub> P	96-900-7297	0.7361



## Search-Match

### Settings

Reference database used	COD-Inorg REV218120 2019.09.10
Automatic zeropoint adaptation	Yes
Minimum figure-of-merit (FoM)	0.60
2theta window for peak corr.	0.30 deg.
Minimum rel. int. for peak corr.	1
Parameter/influence 2theta	0.50
Parameter/influence intensities	0.50
Parameter multiple/single phase(s)	0.50

### Criteria for entries added by user

#### Reference:

**Entry number:** 96-100-1742;96-100-1744;96-101-0918;96-101-0929;96-101-0963;96-210-0993;96-591-0096;96-721-4218;96-721-4219;96-900-0096;96-900-0575;96-900-0966;96-900-0967;96-900-0968;96-900-0969;96-900-0970;96-900-0971;96-900-1298;96-900-1299;96-900-7287;96-900-7688;96-900-7690;96-900-9668;96-900-9669;96-900-9866;96-901-2074;96-901-3466;96-901-4217;96-901-4345;96-901-4393;96-901-4416;96-901-4525;96-901-4612;96-901-4745;96-901-4773;96-901-4878;96-901-4892;96-901-5067;96-901-5074;96-901-5391;96-901-5461;96-901-5482;96-901-5488;96-901-5692;96-901-5762;96-901-5836;96-901-6021;96-901-6023;96-901-6180;96-901-6201;96-901-6465;96-901-6706;96-901-6707;96-100-8767;96-100-8768;96-100-8769;96-101-1088;96-221-1653;96-900-2159;96-900-2160;96-900-3077;96-900-3078;96-900-3079;96-900-3080;96-900-3081;96-901-0407;96-901-0408;96-901-0409;96-901-0410;96-901-0411;96-901-1413;96-901-5697;96-901-6060;96-901-6179;96-901-6407;96-1011046;96-155-0599;96-900-9231;96-900-9235;96-901-5000;96-101-1241;96-101-1268;96-210-8028;96-210-8029;96-591-0083;96-900-0140;96-900-2161;96-900-2162;96-900-2163;96-900-9783;96-901-4881;96-901-5066;96-901-5504;96-901-5965;96-901-6458;96-101-1098;96-101-1160;96-101-1173;96-101-1177;96-101-1201;96-110-0020;96-500-0036;96-900-0776;96-900-0777;96-900-0778;96-900-0779;96-900-0780;96-900-0781;96-900-5018;96-900-5019;96-900-5020;96-900-5021;96-900-5022;96-900-5023;96-900-5024;96-900-5025;96-900-5026;96-900-5027;96-900-5028;96-900-5029;96-900-5030;96-900-5031;96-900-5032;96-900-5033;96-900-5034;96-900-7379;96-900-8093;96-900-8094;96-900-9667;96-901-0145;96-901-0146;96-901-0147;96-901-1494;96-901-1495;96-901-1496;96-901-1497;96-901-2601;96-901-2602;96-901-2603;96-901-2604;96-901-2605;96-901-2606;96-901-3322;96-901-5023

### Peak List

No.	2theta [°]	d [Å]	I/I0	FWHM	Matched
1	11.98	7.3876	373.38	0.2000	
2	14.39	6.1541	931.62	0.3200	A
3	18.24	4.8639	384.02	0.4800	
4	19.50	4.5523	272.67	0.4000	
5	19.94	4.4535	277.41	0.4000	B
6	20.30	4.3747	506.54	1.5600	B
7	20.90	4.2505	541.82	2.4000	B
8	21.34	4.1639	588.16	0.5600	C
9	21.62	4.1105	635.02	0.2800	E
10	21.85	4.0672	152.77	0.6000	B
	23.54	3.7794	366.76	0.2000	B
	25.20	3.5341	196.33	0.3771	B
	27.36	3.2598	419.37	0.2400	B,E
	28.19	3.1656	967.17	0.2800	A
	29.52	3.0260	167.06	0.2555	B,F
	33.24	2.6954	202.89	0.5939	C,D



17	34.68	2.5867	314.14	0.2400	B,C
18	35.26	2.5455	184.38	0.7600	B,C
19	35.72	2.5138	364.90	0.6000	B,C,D
20	36.01	2.4944	280.29	0.4000	B,C,F
21	36.47	2.4640	106.42	3.2800	C
22	37.56	2.3945	170.78	0.4800	B
23	37.93	2.3721	110.91	1.4400	B,E
24	38.35	2.3473	1000.00	0.2800	A,B
25	39.72	2.2693	44.99	0.4336	B,C,F
26	44.86	2.0205	90.43	0.3579	A,B,C
27	45.74	1.9837	121.41	0.3883	A,B
28	47.74	1.9051	262.54	0.3200	B,E,F
29	48.50	1.8770	253.51	0.3600	C
30	48.82	1.8655	704.76	0.3600	A,B,F
31	49.23	1.8510	563.69	0.4000	A,B
32	49.42	1.8442	477.98	0.4000	A,C,D
33	51.32	1.7803	61.41	0.4000	B,C
34	53.56	1.7110	343.14	0.4000	C
35	54.29	1.6897	215.56	1.6400	B,C,D
36	54.67	1.6788	144.31	1.8400	B
37	54.93	1.6716	161.92	1.3200	B
38	55.12	1.6663	494.97	0.3200	A,B,C
39	62.41	1.4880	196.58	0.7200	A,B,D,E
40	62.64	1.4830	176.26	0.6800	B,C,D
41	63.62	1.4626	247.58	0.4400	B,C,F
42	63.96	1.4556	454.69	0.4000	A,B,C,D
43	64.66	1.4416	293.63	0.4800	B,C
44	67.60	1.3858	117.95	0.5670	A,C

## Integrated Profile Areas

### Based on calculated profile

<b>Profile area</b>	<b>Counts</b>	<b>Amount</b>
Overall diffraction profile	116145	100.00%
Background radiation	87902	75.68%
Diffraction peaks	28243	24.32%
Peak area belonging to selected phases	17401	14.98%
<i>Peak area of phase A (Boehmite)</i>	7349	6.33%
<i>Peak area of phase B (Kaolinite)</i>	2872	2.47%
<i>Peak area of phase C (Goethite)</i>	4270	3.68%
<i>Peak area of phase D (Hematite)</i>	1892	1.63%
<i>Peak area of phase E (Quartz)</i>	593	0.51%
<i>Peak area of phase F (Calcite)</i>	426	0.37%
Unidentified peak area	10842	9.33%

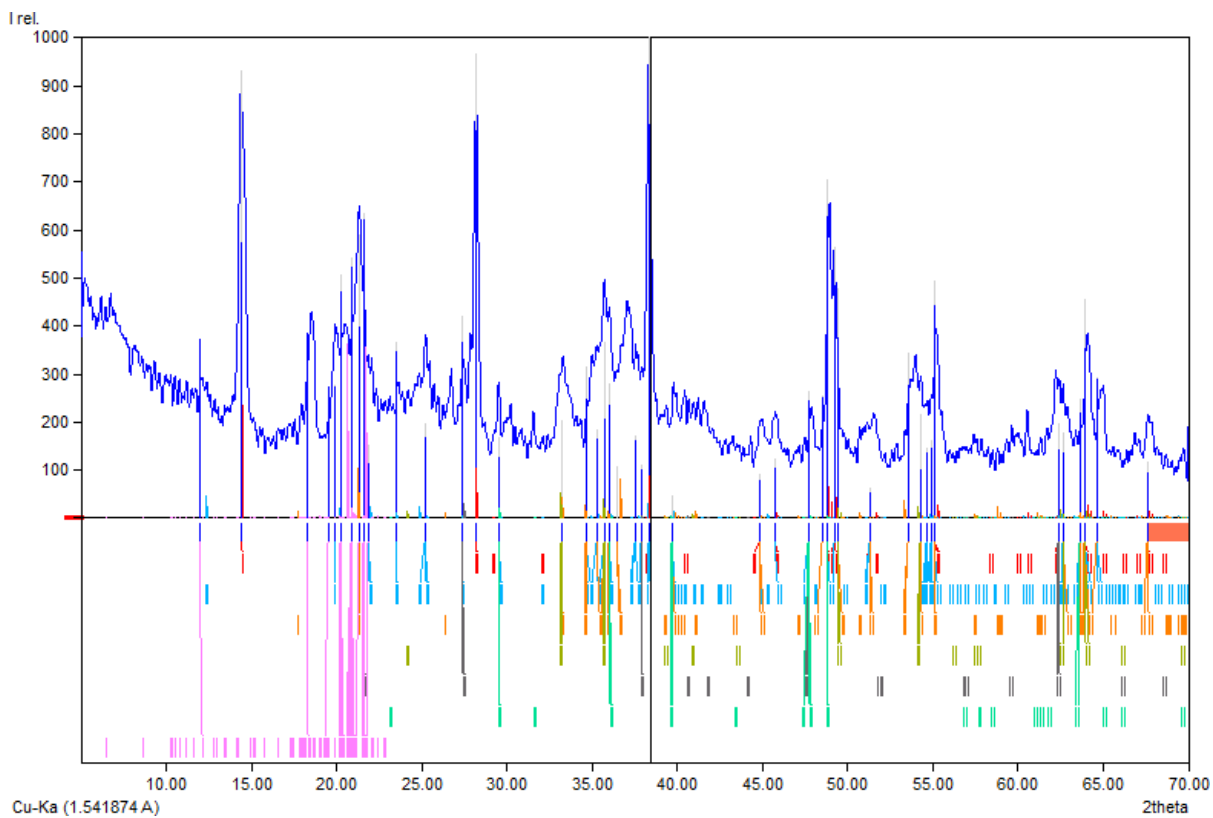
## Peak Residuals

<b>Peak data</b>	<b>Counts</b>	<b>Amount</b>
Overall peak intensity	1160	100.00%
Peak intensity belonging to selected phases	77	6.64%
Unidentified peak intensity	1083	93.36%





## Diffraction Pattern Graphics



Match! Copyright © 2003-2019 CRYSTAL IMPACT, Bonn, Germany



Optimized using  
trial version  
[www.balesio.com](http://www.balesio.com)

# Match! Phase Analysis Report

Sample: R-BTM-3

## SAMPLE DATA

File name R-BTM-3.txt  
 File path D:/RIVALDO XRD/R-BTM-3  
 Data collected Mar 21, 2024 12:09:18  
 Data range 5.000° - 70.000°  
 Original data range 5.000° - 70.000°  
 Number of points 3251  
 Step size 0.020  
 Rietveld refinement converged No  
 Alpha2 subtracted No  
 Background subtr. No  
 Data smoothed Yes  
 Radiation X-rays  
 Wavelength 1.541874 Å

## Matched Phases

Index	Amount (%)	Name	Formula sum
A	40.3	Quartz	O2 Si
B	22.6	Kaolinite	Al2 H4 O9 Si2
C	16.7	Boehmite	Al H O2
D	8.7	Hematite	Fe2 O3
E	8.1	Goethite	Fe H O2
F	3.5	Calcite	C Ca0.871 Mg0.129 O3
	9.4	Unidentified peak area	

### A: QUARTZ (40.3 %)

Formula sum O2 Si  
 Entry number 96-900-0778  
 Figure-of-Merit (FoM) 0.734311  
 Total number of peaks 68  
 Peaks in range 28  
 Peaks matched 12  
 Intensity scale factor 0.32  
 Space group P 32 2 1 S  
 Crystal system trigonal (hexagonal axes)  
 Unit cell a= 4.7736 Å c= 5.3010 Å  
 I/c 3.23  
 Calc. density 2.861 g/cm<sup>3</sup>  
 Reference Levien L., Prewitt C. T., Weidner D. J., "Structure and elastic properties of quartz at pressure P = 37.6 kbar", American Mineralogist **65**, 920-930 (1980)

### B: KAOLINITE (22.6 %)

Formula sum Al2 H4 O9 Si2  
 Entry number 96-900-9231  
 Figure-of-Merit (FoM) 0.495096  
 Total number of peaks 508  
 Peaks in range 262  
 Peaks matched 92  
 Intensity scale factor 0.07  
 Space group C 1  
 Crystal system triclinic (anorthic)  
 Unit cell a= 5.1554 Å b= 8.9448 Å c= 7.4048 Å α= 91.700° β= 104.862°  
 I/c 1.22  
 Calc. density 2.599 g/cm<sup>3</sup>



Reference	Bish D. L., Von Dreele R. B., "Rietveld refinement of non-hydrogen atomic positions in kaoliniteLocality: Keokuk, Iowa, USA", Clays and Clay Minerals <b>37</b> , 289-296 (1989)
<b>C: BOEHMITE (16.7 %)</b>	
Formula sum	Al H O2
Entry number	96-901-2254
Figure-of-Merit (FoM)	0.732928
Total number of peaks	100
Peaks in range	45
Peaks matched	14
Intensity scale factor	0.11
Space group	C m c m
Crystal system	orthorhombic
Unit cell	a= 2.8678 Å b= 12.2188 Å c= 3.6941 Å
l/c	2.76
Calc. density	3.078 g/cm <sup>3</sup>
Reference	Bokhimi X., Toledo-Antonio J A, Guzman-Castillo M L, Hernandez-Beltran F, "Relationship between crystallite size and bond lengths in boehmiteLocality: syntheticSample: preparation T = 240 C", Journal of Solid State Chemistry <b>159</b> , 32-40 (2001)
<b>D: HEMATITE (8.7 %)</b>	
Formula sum	Fe2 O3
Entry number	96-900-0140
Figure-of-Merit (FoM)	0.540418
Total number of peaks	68
Peaks in range	28
Peaks matched	10
Intensity scale factor	0.09
Space group	R -3 c
Crystal system	trigonal (hexagonal axes)
Unit cell	a= 5.0380 Å c= 13.7720 Å
l/c	3.97
Calc. density	5.256 g/cm <sup>3</sup>
Reference	Blake R. L., Hessevick R. E., Zoltai T., Finger L. W., "Refinement of the hematite structure", American Mineralogist <b>51</b> , 123-129 (1966)
<b>E: GOETHITE (8.1 %)</b>	
Formula sum	Fe H O2
Entry number	96-900-2159
Figure-of-Merit (FoM)	0.708821
Total number of peaks	172
Peaks in range	69
Peaks matched	32
Intensity scale factor	0.06
Space group	P n m a
Crystal system	orthorhombic
Unit cell	a= 9.9134 Å b= 3.0128 Å c= 4.5800 Å
l/c	2.93
Calc. density	4.314 g/cm <sup>3</sup>
Reference	Gualtieri A., Venturelli P., "In situ study of the goethite-hematite phase transformation by real timesynchrotron powder diffractionSample at T = 25 C", American Mineralogist <b>84</b> , 895-904 (1999)
<b>TE (3.5 %)</b>	
um	C Ca0.871 Mg0.129 O3



Entry number	96-900-1299
Figure-of-Merit (FoM)	0.623283
Total number of peaks	84
Peaks in range	36
Peaks matched	15
Intensity scale factor	0.03
Space group	R -3 c
Crystal system	trigonal (hexagonal axes)
Unit cell	a= 4.9382 Å c= 16.8320 Å
I/c	3.19
Calc. density	2.748 g/cm <sup>3</sup>
Reference	Paquette J., Reeder R. J., "Single-crystal X-ray structure refinements of two biogenic magnesian calcitecrystalssample LB", American Mineralogist <b>75</b> , 1151-1158 (1990)

### Candidates

<i>Name</i>	<i>Formula</i>	<i>Entry No.</i>	<i>FoM</i>
	Ca Mg <sub>3</sub> N <sub>4</sub> Si	96-400-1936	0.7905
Tb <sub>15</sub> Ni <sub>28</sub> P <sub>21</sub>	Ni <sub>28</sub> P <sub>21</sub> Tb <sub>15</sub>	96-153-6037	0.7883
Eu <sub>4</sub> As <sub>3</sub>	As <sub>3</sub> Eu <sub>4</sub>	96-210-6120	0.7835
Porphyrazinealuminiumchloride	C <sub>16</sub> Al Cl N <sub>16</sub> S <sub>4</sub>	96-430-9965	0.7808
	Y Zn	96-154-1129	0.7649
	C W <sub>2</sub>	96-591-0042	0.7617
(Np Pu)	Np Pu	96-152-2442	0.7596
Bismuth Telluride Selenide (2/2.4/0.6)	Bi <sub>2</sub> Se <sub>0.6</sub> Te <sub>2.4</sub>	96-151-1977	0.7595
Erbium iridium silicide (4/13/9)	Er <sub>4</sub> Ir <sub>13</sub> Si <sub>9</sub>	96-100-8679	0.7592
In <sub>10.2</sub> (Si <sub>12</sub> Al <sub>12</sub> O <sub>48</sub> ) (H <sub>2</sub> S) <sub>0.8</sub>	Al <sub>12</sub> H <sub>1.6</sub> In <sub>10.2</sub> O <sub>48</sub> S <sub>0.8</sub> Si <sub>12</sub>	96-153-1417	0.7579
(Ni (N H <sub>3</sub> )) (C N) <sub>2</sub> (H <sub>2</sub> O) <sub>0.25</sub>	C <sub>2</sub> H <sub>3.5</sub> N <sub>3</sub> Ni O <sub>0.25</sub>	96-153-8520	0.7576
Na Y (C O <sub>3</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>6</sub>	C <sub>2</sub> H <sub>12</sub> Na O <sub>12</sub> Y	96-152-1071	0.7570
Sm <sub>20</sub> Ni <sub>41.6</sub> P <sub>30</sub>	Ni <sub>41.6</sub> P <sub>30</sub> Sm <sub>20</sub>	96-153-6034	0.7565
(Pd <sub>0.2</sub> Zr <sub>0.8</sub> )	Pd <sub>0.2</sub> Zr <sub>0.8</sub>	96-152-2716	0.7552
	Au Yb	96-231-0081	0.7550
(Li Mg)	Li Mg	96-152-2372	0.7549
Adamsite-(Y)	C <sub>2</sub> H <sub>4.89</sub> Ce <sub>0.01</sub> Dy <sub>0.06</sub> Er <sub>0.05</sub> Gd <sub>0.04</sub> Ho <sub>0.02</sub> Na Nd <sub>0.03</sub> O <sub>12</sub> Sm <sub>0.02</sub> Tb <sub>0.01</sub> Tm <sub>0.01</sub> Y <sub>0.72</sub> Yb <sub>0.02</sub>	96-900-4611	0.7549
Zr <sub>2</sub> Pd D <sub>1.70</sub>	D <sub>1.7</sub> Pd Zr <sub>2</sub>	96-153-0331	0.7539
Ba O <sub>2</sub> (H <sub>2</sub> O <sub>2</sub> ) <sub>2</sub>	Ba H <sub>4</sub> O <sub>6</sub>	96-153-9449	0.7534
Alabandite	Mn S	96-900-5939	0.7534
potassium 5-azdotetrazolate	C K N <sub>7</sub>	96-410-3811	0.7530
(In <sub>9.8</sub> H <sub>0.4</sub> ) (Si <sub>12</sub> Al <sub>12</sub> O <sub>48</sub> ) (In S H) <sub>0.4</sub> (H <sub>2</sub> S)	Al <sub>12</sub> H <sub>2.8</sub> In <sub>10.2</sub> O <sub>48</sub> S <sub>1.4</sub> Si <sub>12</sub>	96-153-1414	0.7528
	La <sub>2</sub> Mo <sub>2</sub> O <sub>9</sub>	96-400-0584	0.7527
(Hf <sub>4</sub> Nb <sub>3</sub> Zr <sub>3</sub> ) <sub>0.2</sub>	Hf <sub>0.8</sub> Nb <sub>0.6</sub> Zr <sub>0.6</sub>	96-153-9153	0.7519
Sr <sub>0.935</sub> Fe <sub>4</sub> Sb <sub>12</sub>	Fe <sub>4</sub> Sb <sub>12</sub> Sr <sub>0.935</sub>	96-152-1360	0.7517
	D <sub>1.29</sub> Mg	96-411-1967	0.7510
(Ag <sub>4</sub> ) <sub>2</sub> (N <sub>3</sub> H <sub>5</sub> ) <sub>9</sub> (Si <sub>12</sub> Al <sub>12</sub> O <sub>48</sub> )	Ag <sub>8</sub> Al <sub>12</sub> H <sub>45</sub> N <sub>27</sub> O <sub>48</sub> Si <sub>12</sub>	96-412-4443	0.7510
	Au Tb	96-151-0311	0.7494
	Ag Er	96-150-9304	0.7489
	O <sub>3</sub> S	96-901-1064	0.7475
	Au Er	96-151-0126	0.7471
Uranium-gamma	U	96-900-8557	0.7465
	Hf Sc	96-152-2826	0.7463
Aluminium hydroxide (Gibbsite)	Al H <sub>3</sub> O <sub>3</sub>	96-101-1082	0.7454
Gibbsite	Al O <sub>3</sub>	96-901-5977	0.7454
(Ca P <sub>11</sub> )	Ga Pu	96-152-3831	0.7450
	Au <sub>2</sub> In Pr	96-151-0427	0.7449
	Cl <sub>15</sub> N Zr <sub>6</sub>	96-153-1027	0.7436
	Ba <sub>1.98</sub> Ni <sub>8</sub> Sb <sub>12.24</sub> Sn <sub>11.76</sub>	96-703-9607	0.7433
	Ba <sub>1.57</sub> Ni <sub>8</sub> Sb <sub>16.32</sub> Sn <sub>7.68</sub>	96-703-9604	0.7429
	H <sub>13.64</sub> Mg <sub>4</sub> O <sub>22.82</sub> Si <sub>6</sub>	96-901-5794	0.7428
	Cr F <sub>4</sub> Sr	96-153-4092	0.7427



15

Sepiolite	H12 Mg3.84 O22 Si6	96-901-4920	0.7420
	C20 Cl10 N6	96-151-7089	0.7419
	Ir3 Sc Si7	96-210-6278	0.7419
((Mg Al) (Si4 O10 (H2 O)2 (O H))) (H2 O)2	Al H9 Mg O15 Si4	96-153-3366	0.7417
	U	96-153-9737	0.7417
Tricaesium trioxoantimonate(III)	Cs3 O3 Sb	96-201-2248	0.7416
Ag_zeolite_A	Ag69.45 Al96 O473.69 Si96	96-710-8287	0.7415
Ag_zeolite_A	Ag68.05 Al96 O476.24 Si96	96-710-8288	0.7415
	Au2 Dy2 In	96-720-9405	0.7414
(In9.5 H0.5) (Si12 Al12 O48) (In S H)0.5 (H2 S)2.5 <b>and 4308 others...</b>	Al12 H6 In10 O48 S3 Si12	96-153-1408	0.7413

## Search-Match

### SETTINGS

Reference database used	COD-Inorg REV218120 2019.09.10
Automatic zeropoint adaptation	Yes
Minimum figure-of-merit (FoM)	0.60
2theta window for peak corr.	0.30 deg.
Minimum rel. int. for peak corr.	1
Parameter/influence 2theta	0.50
Parameter/influence intensities	0.50
Parameter multiple/single phase(s)	0.50

### Criteria for entries added by user

#### Reference:

#### Entry number:

96-901-0943;96-901-2248;96-901-2249;96-901-2250;96-901-2251;96-901-2252;96-901-2253;96-901-2254;96-101-1046;96-155-0599;96-900-9231;96-900-9235;96-901-5000;96-101-1241;96-101-1268;96-210-8028;96-210-8029;96-591-0083;96-900-0140;96-900-2161;96-900-2162;96-900-2163;96-900-9783;96-901-4881;96-901-5066;96-901-5504;96-901-5965;96-901-6458;96-101-1098;96-101-1160;96-101-1173;96-101-1177;96-101-1201;96-110-0020;96-500-0036;96-900-0776;96-900-0777;96-900-0778;96-900-0779;96-900-0780;96-900-0781;96-900-5018;96-900-5019;96-900-5020;96-900-5021;96-900-5022;96-900-5023;96-900-5024;96-900-5025;96-900-5026;96-900-5027;96-900-5028;96-900-5029;96-900-5030;96-900-5031;96-900-5032;96-900-5033;96-900-5034;96-900-7379;96-900-8093;96-900-8094;96-900-9667;96-901-0145;96-901-0146;96-901-0147;96-901-1494;96-901-1495;96-901-1496;96-901-1497;96-901-2601;96-901-2602;96-901-2603;96-901-2604;96-901-2605;96-901-2606;96-901-3322;96-901-5023;96-100-8767;96-100-8768;96-100-8769;96-101-1088;96-221-1653;96-900-2159;96-900-2160;96-900-3077;96-900-3078;96-900-3079;96-900-3080;96-900-3081;96-901-0407;96-901-0408;96-901-0409;96-901-0410;96-901-0411;96-901-1413;96-901-5697;96-901-6060;96-901-6179;96-901-6407;96-100-1742;96-100-1744;96-101-0918;96-101-0929;96-101-0963;96-210-0993;96-591-0096;96-721-4218;96-721-4219;96-900-0096;96-900-0575;96-900-0966;96-900-0967;96-900-0968;96-900-0969;96-900-0970;96-900-0971;96-900-1298;96-900-1299;96-900-7287;96-900-7688;96-900-7690;96-900-9668;96-900-9669;96-900-9866;96-901-2074;96-901-3466;96-901-4217;96-901-4345;96-901-4393;96-901-4416;96-901-4525;96-901-4612;96-901-4745;96-901-4773;96-901-4878;96-901-4892;96-901-5067;96-901-5074;96-901-5391;96-901-5461;96-901-5482;96-901-5488;96-901-5692;96-901-5762;96-901-5836;96-901-6021;96-901-6023;96-901-6180;96-901-6201;96-901-6465;96-901-6706;96-901-6707

### Peak List



2theta [°]	d [Å]	I/I0	FWHM	Matched
7.08	12.4857	363.40	0.4000	
8.72	10.1408	291.68	0.2000	
12.00	7.3754	254.31	0.2800	
13.48	6.5688	246.16	0.2400	
14.34	6.1767	397.17	0.3600	C

6	16.24	5.4581	169.72	0.2400	
7	18.16	4.8851	211.14	0.2800	E
8	18.51	4.7930	115.93	0.3600	
9	19.98	4.4440	402.74	0.6000	B
10	20.38	4.3577	376.63	0.6000	B
11	20.94	4.2424	396.40	0.4400	
12	21.48	4.1361	284.17	0.4400	A,B,E
13	23.76	3.7455	506.10	0.2800	B
14	24.62	3.6160	306.58	0.2400	B
15	25.83	3.4493	146.71	0.2400	B
16	26.52	3.3611	273.07	0.2800	B,E
17	26.82	3.3240	84.73	0.7200	
18	27.43	3.2514	1000.00	0.3600	A
19	27.80	3.2092	555.06	0.3600	
20	28.21	3.1639	253.39	0.3200	B,C
21	30.06	2.9729	321.79	0.4000	F
22	30.70	2.9123	271.32	0.3200	
23	33.38	2.6847	50.90	0.8800	D,E
24	35.00	2.5638	417.94	0.4000	B,E
25	35.62	2.5205	428.79	1.1200	B,D,E
26	36.07	2.4900	128.56	2.5600	B,E
27	36.46	2.4644	315.14	2.5200	E,F
28	37.00	2.4296	346.13	0.6400	E
29	38.24	2.3537	401.57	0.4400	B,C
30	41.70	2.1658	239.95	0.2800	A,B,E
31	46.30	1.9610	156.34	0.2400	B
32	47.82	1.9021	195.15	0.3200	B,E,F
33	48.80	1.8662	267.12	0.3600	B,C
34	50.54	1.8060	172.47	0.3200	B
35	50.86	1.7953	300.86	0.3200	B,E
36	53.88	1.7016	118.51	0.5577	B,D,E
37	55.12	1.6663	92.14	0.5645	B,C
38	59.00	1.5656	149.25	0.2400	A,B,E,F
39	62.10	1.4947	312.76	0.4800	A,B,C,D,E,F
40	62.79	1.4798	66.25	0.5600	B,D
41	63.84	1.4581	187.28	0.4000	B,C,D,E,F
42	64.74	1.4400	192.99	0.3600	B,C,E
43	65.80	1.4193	170.24	0.2000	A,B,D,E,F
44	67.60	1.3858	56.10	0.8036	B,C,E

### Integrated Profile Areas

Based on calculated profile

Profile area	Counts	Amount
Overall diffraction profile	130512	100.00%
Background radiation	101975	78.13%
Diffraction peaks	28537	21.87%
Peak area belonging to selected phases	16261	12.46%
Peak area of phase A (Quartz)	4822	3.69%
Peak area of phase B (Kaolinite)	3608	2.76%
Peak area of phase C (Boehmite)	2965	2.27%
Peak area of phase D (Hematite)	2426	1.86%
Peak area of phase E (Goethite)	1977	1.51%
Peak area of phase F (Calcite)	464	0.36%
Total peak area	12276	9.41%

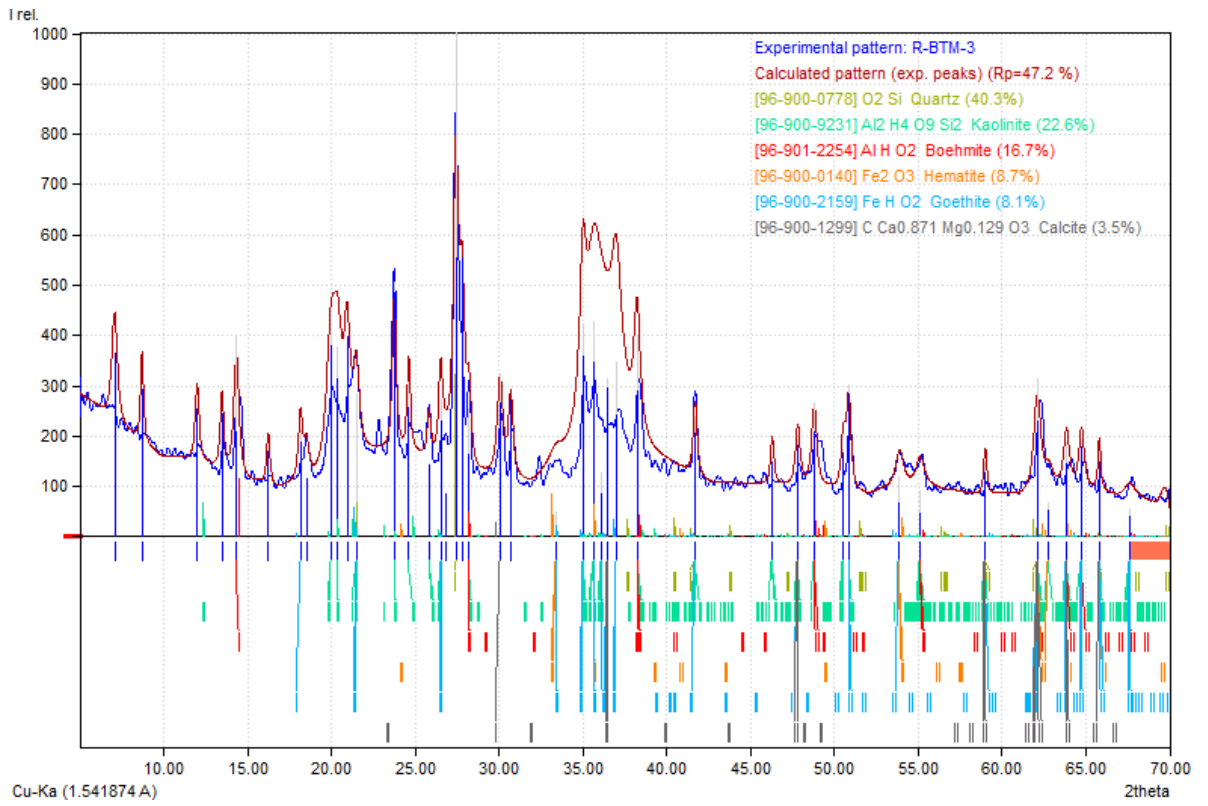


### Peak Residuals

Peak intensity	Counts	Amount
Peak intensity	1141	100.00%

Peak intensity belonging to selected phases	181	15.86%
Unidentified peak intensity	960	84.14%

### Diffraction Pattern Graphics



Match! Copyright © 2003-2019 CRYSTAL IMPACT, Bonn, Germany



Optimized using  
trial version  
[www.balesio.com](http://www.balesio.com)

# Match! Phase Analysis Report

## SAMPLE: R-BTM-4

### Sample Data

File name	R-BTM-4.txt
File path	D:/RIVALDO XRD/R-BTM-4
Data collected	Mar 21, 2024 12:09:18
Data range	5.000° - 70.000°
Original data range	5.000° - 70.000°
Number of points	3251
Step size	0.020
Rietveld refinement converged	No
Alpha2 subtracted	No
Background subtr.	No
Data smoothed	Yes
Radiation	X-rays
Wavelength	1.541874 Å

### MATCHED PHASES

Index	Amount (%)	Name	Formula sum
A	40.4	Boehmite	Al H O2
B	32.7	Kaolinite	Al2 H4 O9 Si2
C	8.5	Calcite	C Ca O3
D	7.9	Hematite	Fe2 O3
E	6.3	Goethite	Fe H O2
F	4.3	Quartz	O2 Si
	10.3	Unidentified peak area	

### A: Boehmite (40.4 %)

Formula sum	Al H O2
Entry number	96-901-2254
Figure-of-Merit (FoM)	0.811091
Total number of peaks	100
Peaks in range	45
Peaks matched	18
Intensity scale factor	0.51
Space group	C m c m
Crystal system	orthorhombic
Unit cell	a= 2.8678 Å b= 12.2188 Å c= 3.6941 Å
I/lc	2.76
Calc. density	3.078 g/cm <sup>3</sup>
Reference	Bokhimi X., Toledo-Antonio J A, Guzman-Castillo M L, Hernandez-Beltran F, "Relationship between crystallitesize and bond lengths in boehmiteLocality: syntheticSample: preparation T = 240 C", Journal of Solid State Chemistry <b>159</b> , 32-40 (2001)

### B: Kaolinite (32.7 %)

Formula sum	Al2 H4 O9 Si2
Entry number	96-900-9235
Merit (FoM)	0.506644
Number of peaks	508
Range	262
Matched	138
Scale factor	0.17
Group	C 1
System	triclinic (anorthic)
	a= 5.1535 Å b= 8.9419 Å c= 7.3906 Å α= 91.926° β= 105.046 °





$\gamma = 89.797^\circ$	
l/c	1.14
Calc. density	2.608 g/cm <sup>3</sup>
Reference	Bish D. L., "Rietveld refinement of the kaolinite structure at 1.5 K Note: sample at T = 1.5 K Locality: Keokuk, Iowa, USA", <i>Clays and Clay Minerals</i> <b>41</b> , 738-744 (1993)

### C: Calcite (8.5 %)

Formula sum	C Ca O3
Entry number	96-900-0970
Figure-of-Merit (FoM)	0.483723
Total number of peaks	86
Peaks in range	36
Peaks matched	19
Intensity scale factor	0.12
Space group	R -3 c
Crystal system	trigonal (hexagonal axes)
Unit cell	a= 4.9780 Å c= 17.4620 Å
l/c	3.09
Calc. density	2.661 g/cm <sup>3</sup>
Reference	Markgraf S. A., Reeder R. J., "High-temperature structure refinements of calcite and magnesite Sample: T = 750 C", <i>American Mineralogist</i> <b>70</b> , 590-600 (1985)

### D: Hematite (7.9 %)

Formula sum	Fe2 O3
Entry number	96-901-6458
Figure-of-Merit (FoM)	0.455172
Total number of peaks	68
Peaks in range	28
Peaks matched	16
Intensity scale factor	0.14
Space group	R -3 c
Crystal system	trigonal (hexagonal axes)
Unit cell	a= 5.0066 Å c= 13.6411 Å
l/c	4.00
Calc. density	5.373 g/cm <sup>3</sup>
Reference	Finger L. W., Hazen R. M., "Crystal structure and isothermal compression of Fe2O3, Cr2O3, and V2O3 to 50kbars Note: P = 43.9 kbar", <i>Journal of Applied Physics</i> <b>51</b> , 5362-5367 (1980)

### E: Goethite (6.3 %)

Formula sum	Fe H O2
Entry number	96-900-3081
Figure-of-Merit (FoM)	0.425538
Total number of peaks	164
Peaks in range	66
Peaks matched	26
Intensity scale factor	0.09
Space group	P b n m
stem	orthorhombic
	a= 4.4683 Å b= 9.8334 Å c= 2.9739 Å
	3.19
sity	4.465 g/cm <sup>3</sup>
›	Nagai T., Kagi H., Yamanaka T., "Variation of hydrogen bonded O. O distances in goethite at high pressure Sample at P = 9.0 GPa", <i>American Mineralogist</i> <b>88</b> , 1423-1427 (2003)



**F: Quartz (4.3 %)**

Formula sum	O2 Si
Entry number	96-900-0776
Figure-of-Merit (FoM)	0.720603
Total number of peaks	70
Peaks in range	31
Peaks matched	22
Intensity scale factor	0.07
Space group	P 32 2 1 S
Crystal system	trigonal (hexagonal axes)
Unit cell	a= 4.9160 Å c= 5.4054 Å
I/lc	3.30
Calc. density	2.646 g/cm <sup>3</sup>
Reference	Levien L., Prewitt C. T., Weidner D. J., "Structure and elastic properties of quartz at pressure P = 1 atm", American Mineralogist <b>65</b> , 920-930 (1980)

**CANDIDATES**

<b>Name</b>	<b>Formula</b>	<b>Entry No.</b>	<b>FoM</b>
	Bi9 Mn5.571 O20.143	96-154-8396	0.8163
	Bi9 Mn5.571 O20.143	96-154-8395	0.8007
	Cu Zr2	96-152-4982	0.8001
Pan004	C48 H96 Bi7 I24 Na3 O12	96-400-2681	0.7979
Poly[(m-2-hydrazine)(m-4-phosphato)iron(III)]	Fe H4 N2 O4 P	96-224-1301	0.7961
Retgersite	Ni O10 S	96-901-1290	0.7952
Carlinite	S Ti2	96-901-2278	0.7946
Calcium	Ca	96-901-2917	0.7934
Jonesite	Al2 Ba4 H22 K1.6 Na0.4 O41.02 Si10 Ti4	96-900-3317	0.7932
	B2 H4 O4	96-705-0580	0.7928
	B H2 O2	96-901-6430	0.7928
	Co H4 N2 O4 S	96-432-4099	0.7923
	Mn5 O24 S6 Sr	96-150-8819	0.7913
Sr2 Zn (Ge2 O7)	Ge2 O7 Sr2 Zn	96-153-6208	0.7911
(Np Pu)	Np Pu	96-152-2442	0.7901
Acetylene dicarboxylic acid dihydrate	C4 H6 O6	96-590-0036	0.7899
Retgersite	H12 Ni O10 S	96-901-1289	0.7886
	C36 H88 Ge12 Nd8 O68	96-410-5261	0.7878
	Li2 Mo O4	96-702-4043	0.7875
	C4 N5 S3	96-411-6295	0.7873
?La2O2Zn0.1Mn0.9Se2?	La2 Mn0.9 O2 Se2 Zn0.1	96-434-2931	0.7873
	C6 H20 Cl4 Mn N2	96-210-1147	0.7865
	C12 F8 Hg N2 O4	96-720-5217	0.7849
Ag6 (Ge O4) (S O4)	Ag6 Ge O8 S	96-810-3412	0.7843
	Hf	96-153-9077	0.7835
Martinite	B2.84 Ca4.58 F2 H5.96 Na9.34 O44	96-901-0638	0.7830
	Si13.16		
Na Y (C O3)2 (H2 O)6	C2 H12 Na O12 Y	96-152-1071	0.7822
	Al2 Na2.28 O8 Si2	96-400-2835	0.7815
trizinc borate phosphate	B O7 P Zn3	96-222-8902	0.7809
Hafnium	Hf	96-900-8502	0.7797
Li Na5 (P O4)2	Li Na5 O8 P2	96-153-4957	0.7793
	Co Ge2 O7 Sr2	96-432-8649	0.7792
	Hf	96-151-2511	0.7781
Sm (V O4)	O4 Sm V	96-152-7827	0.7780
antimony oxide	Ni O3 Ti	96-101-0027	0.7778
	Ni O3 Ti	96-900-8037	0.7778
	C4 H12 Al5 F17 N10	96-450-6127	0.7777
tantanium indium phosphate			
5/.15/3)	C4 H12 Al5 F17 N10	96-100-8368	0.7769
	1.15 O12 P3 Ti1.85		



96-100-8368			
0.7769			
Li <sub>2</sub> (Te O <sub>3</sub> )	Li <sub>2</sub> O <sub>3</sub> Te	96-153-7118	0.7768
gadolinium orthovanadate	Gd O <sub>4</sub> V	96-434-1677	0.7768
Trivanadium(III) silicopentaphosphate	O <sub>19</sub> P <sub>5</sub> Si V <sub>3</sub>	96-100-1684	0.7766
Gainesite	Be <sub>0.5</sub> Na <sub>0.956</sub> O <sub>8</sub> P <sub>2</sub> Zr	96-900-0904	0.7765
Adamsite-(Y)	C <sub>2</sub> H <sub>4.89</sub> Ce <sub>0.01</sub> Dy <sub>0.06</sub> Er <sub>0.05</sub> Gd <sub>0.04</sub> Ho <sub>0.02</sub> Na Nd <sub>0.03</sub> O <sub>12</sub> Sm <sub>0.02</sub> Tb <sub>0.01</sub> Tm <sub>0.01</sub> Y <sub>0.72</sub> Yb <sub>0.02</sub>	96-900-4611	0.7765
H <sub>8</sub> Pt O <sub>6</sub>	H <sub>8</sub> O <sub>6</sub> Pt	96-152-7115	0.7762
Carlinite	S Ti <sub>2</sub>	96-901-1852	0.7761
(Li <sub>1.45</sub> Na <sub>0.45</sub> ) (Ti <sub>1.1</sub> Al <sub>0.9</sub> ) (P O <sub>4</sub> ) <sub>3</sub>	Al <sub>0.9</sub> Li <sub>1.45</sub> Na <sub>0.45</sub> O <sub>12</sub> P <sub>3</sub> Ti <sub>1.1</sub>	96-722-1289	0.7759
tetrachloro-o-benzoquinone	C <sub>6</sub> Cl <sub>4</sub> O <sub>2</sub>	96-151-6179	0.7751
	Ga <sub>3</sub> Y <sub>5</sub>	96-152-8256	0.7750
	Pb <sub>5</sub> Sr <sub>3</sub>	96-151-8045	0.7740
	Cr <sub>0.5</sub> Li <sub>2</sub> O <sub>3</sub> Sb <sub>0.5</sub>	96-703-0803	0.7739
Ammonium hexafluorosilicate (Cryptohalite)	F <sub>6</sub> H <sub>8</sub> N <sub>2</sub> Si	96-101-0993	0.7738
Cryptohalite	F <sub>6</sub> N <sub>2</sub> Si	96-901-6697	0.7738
and 9950 others...			

## SEARCH-MATCH

### Settings

Reference database	COD-Inorg REV218120 2019.09.10
used	Automatic zeropoint
adaptation	Yes
Minimum figure-of-merit (FoM)	0.31
2theta window for peak corr.	0.30 deg.
Minimum rel. int. for peak corr.	1
Parameter/influence 2theta	0.50
Parameter/influence intensities	0.50
Parameter multiple/single phase(s)	0.50

## CRITERIA FOR ENTRIES ADDED BY USER

### Reference:

#### Entry number:

96-100-1742;96-100-1744;96-101-0918;96-101-0929;96-101-0963;96-210-0993;96-591-0096;96-721-4218;96-721-4219;96-900-0096;96-900-0575;96-900-0966;96-900-0967;96-900-0968;96-900-0969;96-900-0970;96-900-0971;96-900-1298;96-900-1299;96-900-7287;96-900-7688;96-900-7690;96-900-9668;96-900-9669;96-900-9866;96-901-2074;96-901-3466;96-901-4217;96-901-4345;96-901-4393;96-901-4416;96-901-4525;96-901-4612;96-901-4745;96-901-4773;96-901-4878;96-901-4892;96-901-5067;96-901-5074;96-901-5391;96-901-5461;96-901-5482;96-901-5488;96-901-5692;96-901-5762;96-901-5836;96-901-6021;96-901-6023;96-901-6180;96-901-6201;96-901-6465;96-901-6706;96-901-6707;96-101-1046;96-155-0599;96-900-9231;96-900-9235;96-901-5000;96-101-1241;96-101-1268;96-210-8028;96-210-8029;96-591-0083;96-900-0140;96-900-2161;96-900-2162;96-900-2163;96-900-9783;96-901-4881;96-901-5066;96-901-5504;96-901-5965;96-901-6458;96-100-8767;96-100-8768;96-100-8769;96-101-1088;96-221-1653;96-900-2159;96-900-2160;96-900-3077;96-900-3078;96-900-3079;96-900-3080;96-900-3081;96-901-0407;96-901-0408;96-901-0409;96-901-0410;96-901-0411;96-901-1413;96-901-5697;96-901-6060;96-901-6179;96-901-6407



## PEAK LIST

No.	2theta [°]	d [Å]	I/I0	FWHM	Matched
1	6.36	13.8975	678.98	0.2400	
2	6.88	12.8483	707.56	0.2800	
3	13.46	6.5785	377.03	0.2000	
4	14.42	6.1426	1000.00	0.4400	A
5	18.40	4.8219	484.46	0.3600	
6	19.76	4.4930	488.51	0.6000	B
7	20.66	4.2986	203.67	1.9600	B
8	20.96	4.2384	587.06	0.6000	F
9	21.28	4.1754	723.11	0.6000	B
10	24.20	3.6778	402.08	0.2400	D
11	24.54	3.6276	463.77	0.4000	
12	25.18	3.5368	519.26	0.4000	B
13	26.58	3.3537	471.91	0.3200	B,F
14	27.33	3.2632	717.99	0.2800	
15	28.21	3.1636	680.82	0.3200	A,B
16	29.42	3.0358	782.68	0.3200	C
17	29.90	2.9884	353.93	0.3200	
18	30.88	2.8962	89.62	0.6000	C
19	31.46	2.8437	311.76	0.2400	B
20	32.14	2.7851	322.63	0.4400	
21	32.94	2.7192	428.76	0.6000	B
22	34.56	2.5954	379.12	0.2000	
23	35.00	2.5638	527.17	0.4400	B,E
24	35.52	2.5274	725.52	0.8400	B,E
25	36.72	2.4472	150.45	1.8400	E,F
26	37.02	2.4284	564.22	1.0000	
27	38.35	2.3470	727.85	0.3200	A,B
28	39.43	2.2855	182.67	0.2800	B,C,D,F
29	39.82	2.2638	398.51	0.2800	B,D
30	40.48	2.2284	361.15	0.3200	B,E,F
31	41.22	2.1901	148.67	0.6582	B,D,E
32	43.21	2.0937	151.33	0.2800	B,C
33	44.80	2.0231	306.12	0.3600	A,E
34	45.48	1.9944	279.59	0.4400	B,F
35	47.57	1.9115	197.95	0.2800	B
36	48.11	1.8913	65.36	2.0400	B,C,E
37	48.50	1.8770	496.15	0.3600	
38	48.92	1.8618	490.74	0.8800	A,B
39	49.24	1.8504	386.63	0.4400	A,B,E
40	49.88	1.8283	234.70	0.4400	B,D,F
41	50.58	1.8046	222.66	0.3200	B,E,F
42	51.26	1.7823	283.81	0.3600	B
43	54.04	1.6970	444.09	0.8400	B
44	54.48	1.6843	385.27	1.7600	B,D,E
45	55.19	1.6642	275.00	0.4000	A,B,F
46	56.62	1.6256	251.47	0.2000	B,C,D
47	57.34	1.6069	304.53	0.4400	B,C,F
48	61.22	1.5140	279.70	0.2800	B
49	61.78	1.5017	285.47	0.4400	B
50	62.22	1.4921	421.98	0.4400	A,B,E
51	62.91	1.4774	83.99	0.7600	B,C,D,E
52	63.94	1.4560	423.45	0.3600	B,C,F
53	64.32	1.4484	378.34	0.3600	A,B,D,E,F
54	64.78	1.4392	409.48	0.3600	A,B,C,D,E
55	67.60	1.3858	96.60	0.4562	A,B,F



## Integrated Profile Areas

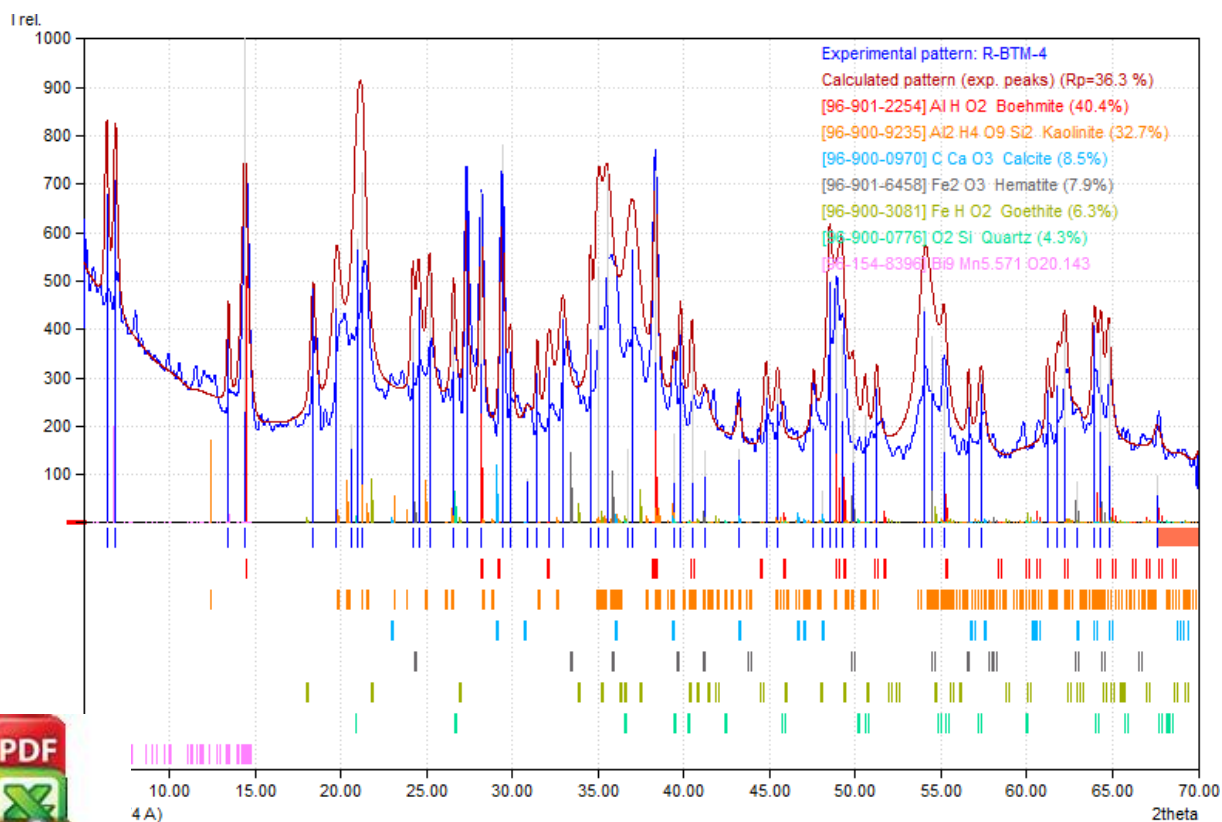
### Based on calculated profile

<b>Profile area</b>	<b>Counts</b>	<b>Amount</b>
Overall diffraction profile	118821	100.00%
Background radiation	92803	78.10%
Diffraction peaks	26018	21.90%
Peak area belonging to selected phases	13807	11.62%
Peak area of phase A (Boehmite)	5582	4.70%
Peak area of phase B (Kaolinite)	3677	3.09%
Peak area of phase C (Calcite)	745	0.63%
Peak area of phase D (Hematite)	1971	1.66%
Peak area of phase E (Goethite)	1422	1.20%
Peak area of phase F (Quartz)	410	0.35%
Unidentified peak area	12211	10.28%

## PEAK RESIDUALS

<b>Peak data</b>	<b>Counts</b>	<b>Amount</b>
Overall peak intensity	1009	100.00%
Peak intensity belonging to selected phases	366	36.30%
Unidentified peak intensity	643	63.70%

## Diffraction Pattern Graphics



Match! Copyright © 2003-2019 CRYSTAL IMPACT, Bonn, Germany

Optimized using  
 trial version  
[www.balesio.com](http://www.balesio.com)

## Lampiran 4 Hasil Analisis XRF



Optimized using  
trial version  
[www.balesio.com](http://www.balesio.com)



## SUPERINTENDING COMPANY OF INDONESIA



SAMPLE ID	SiO <sub>2</sub>	Al <sub>2</sub> O <sub>3</sub>	TiO <sub>2</sub>	Fe <sub>2</sub> O <sub>3</sub>	CaO
RBTM-1	17.08	34.04	1.53	14.19	5.44
RBTM-2	15.22	39.16	1.70	16.15	1.50
RBTM-3	27.29	29.62	1.23	11.21	2.24
RBTM-4	15.93	33.47	1.50	13.83.	5.30



## Lampiran 5 Kartu Konsultasi Tugas Akhir





**Lampiran B 10**  
**Kartu Konsultasi Tugas Akhir**

**JUDUL: KARAKTERISASI BIJIH BAUKSIT KARST DAERAH BANTIMURU  
KABUPATEN MAROS, SULAWESI SELATAN**

(Konsultasi minimal 8 kali)

TANGGAL	MATERI KONSULTASI	PARAF DOSEN
26/04/2024	- Judul Penelitian - Abstrak - Tujuan Penelitian	A
29/04/2024	- Penulisan rumus Kimia - Peta Penelitian - Saran Penelitian	A
02/05/2024	- Hasil analisis Mikroskopis - Hasil XRD - Penulisan bahasa Inggris	A
03/05/2024	- Grafik difraktogram XRD - Kesimpulan - Diagram alir Penelitian	A
2024	- Poster Ilmiah - Artikel Ilmiah	A



TANGGAL	MATERI KONSULTASI	PARAF DOSEN
07/05/2024	- Artikel ilmiah - Peta penelitian	WF
08/05/2024	- Artikel ilmiah	A
08/05/2024	Acc untuk seminar hasil	A
24/06/2024	- Asistensi tugas pustaka - Peta Penelitian	A
24/06/2024		A

